MATERIAL DATA SHEET

# RadonPy PI222, polystyrene family amorphous MD model

Open RadonPy computational screening card for a polystyrene family repeat unit with available amorphous-state physical, thermal, mechanical, dielectric, and optical predictions.

| Field | Value |
|---|---|
| Material ID | radonpy-pi222 |
| Category | Polymer |
| Condition | amorphous homopolymer computational model \| periodic molecular-dynamics cell |
| Unit system | Common SI |
| Unit contract | Material properties stored in SI engineering units. |
| Generated | 2026-11-15 22:57 |

## Source and Validity

| Field | Value |
|---|---|
| Quality | Computational screening |
| Design release allowed | No |
| Source family | Computational dataset |
| Confidence | Engineering estimate |
| License | Open |
| Source note | BSD-3-Clause RadonPy computed amorphous-polymer record generated from a pinned, hash-checked CSV; no PoLyInfo experimental validation values are included. |
| Citation | RadonPy PI1070 calculated dataset, commit 840dd4a2b5f261fc9370bb6786eff0b71a463d2f, record PI222, BSD-3-Clause; method DOI 10.1038/s41524-022-00906-4; https://github.com/RadonPy/RadonPy |
| Valid temperature | 300 ... 300 K (Single modeled temperature in the pinned PI1070 CSV.) |
| Valid pressure | 1 ... 1 atm (Upstream pressure input under the LAMMPS real-unit convention.) |
| Valid phase / condition | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Uncertainty | Classical MD screening result, not a measured grade datasheet. The method paper reports property-dependent bias/correlation limitations; additives, crystallinity, cure, aging, processing, and commercial-grade variation are not represented. |
| Last reviewed | 2026-07-30 |
| Reviewer | scripts/import_radonpy_public_polymers.py |
| Review status | Checked |

| Field | Value |
|---|---|
| Review scope | Checked pinned hashes, BSD attribution, CSV field units, row count, deterministic conversions, and exclusion of PoLyInfo experimental data; not validated for engineering release. |
| Notes | Computational homopolymer structure, not a supplier grade or formulation. |
| License ID | BSD-3-Clause |
| License URL | https://opensource.org/license/bsd-3-clause |
| Attribution | RadonPy developers; Hayashi et al., npj Computational Materials 8, 222 (2022) |

## Material Condition

| Field | Value |
|---|---|
| Condition | amorphous homopolymer computational model |
| Product form | periodic molecular-dynamics cell |
| Thickness / diameter range | Not applicable to the computational cell. |
| Test direction | Bulk isotropic modeled response. |
| Processing route | RadonPy automated all-atom classical molecular-dynamics workflow. |
| Temperature range | 300 ... 300 K |
| Notes | Classical MD screening result, not a measured grade datasheet. The method paper reports property-dependent bias/correlation limitations; additives, crystallinity, cure, aging, processing, and commercial-grade variation are not represented. |

## Properties

## Physical

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Density | 1094.086295 | kg/m^3 | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |

## Thermal

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Specific heat capacity, cp | 2791.647421 | J/kg/K | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Specific heat capacity, cv | 2759.464748 | J/kg/K | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Volumetric thermal expansion coefficient | 0.000109667 | 1/K | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Linear thermal expansion coefficient | 3.66e-05 | 1/K | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Thermal conductivity | 0.16724356 | W/m/K | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Thermal diffusivity | 5.5e-08 | m^2/s | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |

## Mechanical

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Bulk modulus | 1.503036154 | GPa | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Isentropic bulk modulus | 1.523855226 | GPa | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |

## Electrical

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Static dielectric constant, dipole-fluctuation term | 1.468733288 | - | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Static dielectric constant, electronic-corrected | 2.703552779 | - | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |

## Identity

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Repeat-unit SMILES | *C(C(*)c1ccccc1)[N+](=O)[O-] | - | Model Input | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| RadonPy polymer class | 2: polystyrene family | - | Computed Classification | RadonPy structural classification of the repeat-unit SMILES. |

## Model

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Number-average molecular mass | 8233.265 | g/mol | Model Input | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |
| Degree of polymerization | 55 | - | Model Input | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |

## Optical

| Property | Value | Unit | Type | Applies to |
|---|---|---|---|---|
| Refractive index | 1.494894075 | - | Computed Mean | RadonPy amorphous homopolymer MD model at 300 K and upstream press=1 (LAMMPS real-unit atmosphere); tacticity=atactic, degree of polymerization=55. |

Engineering note: seed solid-material values are reference values only. Verify against the project material specification or supplier data sheet before release.