

Beta-cyanostyrene

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| Other names: | cinnamotrile |
| Inchi: | InChI=1S/C9H7N/c10-8-4-7-9-5-2-1-3-6-9/h1-7H |
| InchiKey: | ZWKNLRFUTWSOY-UHFFFAOYSA-N |
| Formula: | C9H7N |
| SMILES: | N#CC=Cc1cccc1 |
| Mol. weight [g/mol]: | 129.16 |
| CAS: | 4360-47-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 350.71 | kJ/mol | Joback Method |
| hf | 289.54 | kJ/mol | Joback Method |
| hfus | 14.81 | kJ/mol | Joback Method |
| hvap | 48.34 | kJ/mol | Joback Method |
| log10ws | -2.58 | | Crippen Method |
| logp | 2.223 | | Crippen Method |
| mcvol | 110.990 | ml/mol | McGowan Method |
| pc | 3364.54 | kPa | Joback Method |
| tb | 538.24 | K | Joback Method |
| tc | 776.63 | K | Joback Method |
| tf | 277.52 | K | Joback Method |
| vc | 0.438 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 225.13 | J/mol×K | 538.24 | Joback Method |
| cpg | 235.97 | J/mol×K | 577.97 | Joback Method |
| cpg | 245.97 | J/mol×K | 617.70 | Joback Method |
| cpg | 255.18 | J/mol×K | 657.44 | Joback Method |
| cpg | 263.67 | J/mol×K | 697.17 | Joback Method |
| cpg | 271.49 | J/mol×K | 736.90 | Joback Method |
| cpg | 278.72 | J/mol×K | 776.63 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C4360478&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| h vap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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