1-Phenylcyclopentanenitrile

Other names: 1-Phenyl-1-cyclopentanecarbonitrile
Cyclopentanecarbonitrile, 1-phenyl-
1-Phenylcyclopentanecarbonitrile
1-phenylcyclohexanecarbonitrile
Inchi: InChI=1S/C12H13N/c13-10-12(8-4-5-9-12)11-6-2-1-3-7-11/h1-3,6-7H,4-5,8-9H2
InchiKey: GDXMFFGTPGAGGX-UHFFFAOYSA-N
Formula: C12H13N
SMILES: N#CC1(c2ccccc2)CCCC1
Mol. weight [g/mol]: 171.24
CAS: 77-57-6

Physical Properties

Property code	Value	Unit	Source
gf	326.81	kJ/mol	Joback Method
hf	186.12	kJ/mol	Joback Method
hfus	10.02	kJ/mol	Joback Method
hvap	54.17	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.022		Crippen Method
mcvol	146.700	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
tb	618.24	K	Joback Method
tc	876.13	K	Joback Method
tf	351.21	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.17	J/mol×K	618.24	Joback Method
cpg	383.23	J/mol×K	661.22	Joback Method
cpg	398.10	J/mol×K	704.20	Joback Method
cpg	412.02	J/mol×K	747.18	Joback Method
cpg	425.22	J/mol×K	790.17	Joback Method

cpg	437.93	J/mol×K	833.15	Joback Method
cpg	450.39	J/mol×K	876.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.70	K	1.30	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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=C77576&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
hvap: 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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume