

1-PIPERIDINOCYCLOHEXANE CARBONITRILE

Other names:	Cyclohexanecarbonitrile, 1-piperidino- 1-Piperidinocyclohexanecarbonitrile 1-(1-Cyanocyclohexyl)piperidine PCC Piperidinocyclohexanecarbonitrile
Inchi:	InChI=1S/C12H20N2/c13-11-12(7-3-1-4-8-12)14-9-5-2-6-10-14/h1-10H2
InchiKey:	WWSAYKJWUZJLRT-UHFFFAOYSA-N
Formula:	C12H20N2
SMILES:	N#CC1(N2CCCCC2)CCCCC1
Mol. weight [g/mol]:	192.31

Physical Properties

Property code	Value	Unit	Source
chs	-7496.18 ± 0.37	kJ/mol	NIST Webbook
hf	3.53 ± 0.77	kJ/mol	NIST Webbook
hfs	-84.23 ± 0.44	kJ/mol	NIST Webbook
hsub	87.76 ± 0.63	kJ/mol	NIST Webbook
hsub	87.80	kJ/mol	NIST Webbook
hsub	87.80 ± 0.60	kJ/mol	NIST Webbook
logp	2.699		Crippen Method
mcvol	169.580	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.44	kJ/mol	339.20	NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3867150&Units=SI>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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