

2-Dimethylaminomethyl-1-(2'-piperidylmethyl)-cyclohexane

Inchi:	InChI=1S/C15H30N2O/c1-17(2)12-13-7-3-5-9-15(13,18)11-14-8-4-6-10-16-14/h13-14,16
InchiKey:	IXHYXGISKEYIS-UHFFFAOYSA-N
Formula:	C15H30N2O
SMILES:	CN(C)CC1CCCCC1(O)CC1CCCCN1
Mol. weight [g/mol]:	254.41
CAS:	116373-16-1

Physical Properties

Property code	Value	Unit	Source
gf	172.79	kJ/mol	Joback Method
hf	-296.28	kJ/mol	Joback Method
hfus	29.75	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.002		Crippen Method
mcvol	226.320	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	730.44	K	Joback Method
tc	942.22	K	Joback Method
tf	491.55	K	Joback Method
vc	0.812	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.70	J/mol×K	730.44	Joback Method
cpg	744.17	J/mol×K	765.74	Joback Method
cpg	764.56	J/mol×K	801.03	Joback Method
cpg	784.00	J/mol×K	836.33	Joback Method
cpg	802.61	J/mol×K	871.63	Joback Method
cpg	820.51	J/mol×K	906.93	Joback Method
cpg	837.83	J/mol×K	942.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116373161&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
mccvol:	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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