2-Adamantylamine, N,N-dimethyl-

Other names: 2-N,N-dimethylamino-adamantane
Inchi: InChI=1S/C12H21N/c1-13(2)12-10-4-8-3-9(6-10)7-11(12)5-8/h8-12H,3-7H2,1-2H3
InchiKey: LGQPYDNHZPYIRL-UHFFFAOYSA-N
Formula: C12H21N
SMILES: CN(C)C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 179.30

Physical Properties

Property code	Value	Unit	Source
gf	315.67	kJ/mol	Joback Method
hf	-51.92	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	43.64	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.373		Crippen Method
mcvol	157.340	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1409.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1365.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1365.00		NIST Webbook
tb	501.55	K	Joback Method
tc	706.14	K	Joback Method
tf	299.29	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.65	J/mol×K	501.55	Joback Method
cpg	426.62	J/mol×K	535.65	Joback Method
cpg	448.12	J/mol×K	569.75	Joback Method

cpg	468.24	J/mol×K	603.85	Joback Method
cpg	487.06	J/mol×K	637.94	Joback Method
cpg	504.69	J/mol×K	672.04	Joback Method
cpg	521.20	J/mol×K	706.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374752&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume