

1-Adamantanamine, N,N-dimethyl-

Other names:	(Dimethylamino)adamantane N,N-Dimethyl-1-adamantylamine 1-(Dimethylamino)adamantane N,N-Dimethyl-1-adamantanamine Tricyclo(3.3.1.1)
Inchi:	InChI=1S/C12H21N/c1-13(2)12-6-9-3-10(7-12)5-11(4-9)8-12/h9-11H,3-8H2,1-2H3
InchiKey:	NFBYCNFAXLUGBT-UHFFFAOYSA-N
Formula:	C12H21N
SMILES:	CN(C)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	179.30
CAS:	3717-40-6

Physical Properties

Property code	Value	Unit	Source
gf	317.89	kJ/mol	Joback Method
hf	-16.34	kJ/mol	Joback Method
hfus	16.94	kJ/mol	Joback Method
hvap	42.80	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.517		Crippen Method
mcvol	157.340	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	506.46	K	Joback Method
tc	719.91	K	Joback Method
tf	327.43	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.93	J/mol×K	506.46	Joback Method
cpg	426.60	J/mol×K	542.03	Joback Method
cpg	447.54	J/mol×K	577.61	Joback Method
cpg	466.95	J/mol×K	613.18	Joback Method

cpg	485.00	J/mol×K	648.76	Joback Method
cpg	501.90	J/mol×K	684.33	Joback Method
cpg	517.83	J/mol×K	719.91	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=C3717406&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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