1-Adamantanemethylamine, «alpha»-methyl-

Other names:	(dl)-rimantadine
	.alpha.-methyltricyclo[3.3.1.1(3,7)]decane-1-methanamine
	1-(adamantan-1-yl)ethan-1-amine
	Rimantadine
	Tricyclo(3.3.1.1
	«alpha»-Methyl-1-adamantanemethylamine
	«alpha»-Methyladamantanemethylamine
Inchi:	InChI=1S/C12H21N/c1-8(13)12-5-9-2-10(6-12)4-11(3-9)7-12/h8-11H,2-7,13H2,1H3
InchiKey:	UBCHPRBFMUDMNC-UHFFFAOYSA-N
Formula:	C12H21N
SMILES:	CC(N)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	179.30
CAS:	13392-28-4

Physical Properties

Property code	Value	Unit	Source
gf	271.12	kJ/mol	Joback Method
hf	-55.36	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.550		Crippen Method
mcvol	157.340	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
tb	566.11	K	Joback Method
tc	797.40	K	Joback Method
tf	363.22	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.95	J/mol×K	566.11	Joback Method
cpg	462.18	J/mol×K	604.66	Joback Method

cpg	481.81	J/mol×K	643.21	Joback Method
cpg	500.10	J/mol×K	681.76	Joback Method
cpg	517.27	J/mol×K	720.30	Joback Method
cpg	533.55	J/mol×K	758.85	Joback Method
cpg	549.18	J/mol×K	797.40	Joback Method
pvap	3.00e-03	kPa	298.15	The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography

Sources

The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je400498a
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=C13392284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume