Amantadine

Other names:	1-Adamantamine
	1-Adamantanamine
	1-Adamantylamine
	1-Aminoadamantane
	1-Aminotricyclo(3.3.1.1
	1-aminotricyclo(3.3.1.1:3,7)decane
	Adamantamine
	Adamantanamine
	Adamantylamine
	Aminoadamantane
	Pk-Merz
	Tricyclo[3.3.1.1(3,7)]decan-1-amine
	sulfasalazine
	tricyclo(3.3.1.1:3,7)decan-1-amine
Inchi:	InChI=1S/C10H17N/c11-10-4-7-1-8(5-10)3-9(2-7)6-10/h7-9H,1-6,11H2
InchiKey:	DKNWSYNQZKUICI-UHFFFAOYSA-N
Formula:	C10H17N
SMILES:	NC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	151.25
CAS:	768-94-5

Physical Properties

Property code	Value	Unit	Source
affp	948.80	kJ/mol	NIST Webbook
basg	916.30	kJ/mol	NIST Webbook
gf	256.72	kJ/mol	Joback Method
hf	-8.80	kJ/mol	Joback Method
hfus	7.30	kJ/mol	The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography
hfus	1.72	kJ/mol	Thermodynamic properties of 1-aminoadamantane
hsub	61.70 ± 0.60	kJ/mol	NIST Webbook
hvap	46.95	kJ/mol	Joback Method

log10ws	-6.14		Aqueous Solubility Prediction Method
logp	1.914		Crippen Method
mcvol	129.160	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1240.00		NIST Webbook
tb	520.79	K	Joback Method
tc	755.79	K	Joback Method
tf	355.68	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.21	J/mol×K	520.79	Joback Method
cpg	362.22	J/mol×K	559.96	Joback Method
cpg	380.54	J/mol×K	599.12	Joback Method
cpg	397.41	J/mol×K	638.29	Joback Method
cpg	413.05	J/mol×K	677.45	Joback Method
cpg	427.71	J/mol×K	716.62	Joback Method
cpg	441.62	J/mol×K	755.79	Joback Method

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
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C768945&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic properties of 1-aminoadamantane:	https://www.doi.org/10.1016/j.jct.2007.08.002
Thermodynamics of the Antiviral and Antiparkinsonian Drug Amantadine Hydrochloride: Condensed State Properties and Decomposition:	https://www.doi.org/10.1021/acs.jced.7b00107

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hsub:	Enthalpy of sublimation 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