

1-ADAMANTANEMETHYLAMINE

Other names:	Tricyclo[3.3.1.1(3,7)-]decane-1-methanamine tricyclo[3.3.1.13,7]dec-1-ylmethylamine
Inchi:	InChI=1S/C11H19N/c12-7-11-4-8-1-9(5-11)3-10(2-8)6-11/h8-10H,1-7,12H2
InchiKey:	XSOHXMFFSKTSIT-UHFFFAOYSA-N
Formula:	C11H19N
SMILES:	NCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	165.28

Physical Properties

Property code	Value	Unit	Source
hfus	16.52	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.45		Cheméo Relay (1.0)
logp	2.162		Crippen Method
mcvol	143.250	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.69	J/mol×K	543.67	Joback Method
cpg	411.07	J/mol×K	582.09	Joback Method
cpg	429.86	J/mol×K	620.52	Joback Method
cpg	447.27	J/mol×K	658.94	Joback Method
cpg	463.53	J/mol×K	697.36	Joback Method
cpg	478.88	J/mol×K	735.79	Joback Method
cpg	493.53	J/mol×K	774.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.20	K	0.04	NIST Webbook

tbrp	357.00 ± 1.00	K	0.04	NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17768411&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
tbrp:	Boiling point at reduced pressure

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