

1-Methyl-3-ethyladamantane

Other names:	1-Ethyl-3-methyladamantane
Inchi:	InChI=1S/C13H22/c1-3-13-7-10-4-11(8-13)6-12(2,5-10)9-13/h10-11H,3-9H2,1-2H3
InchiKey:	HUCLCMAVGXHPPK-UHFFFAOYSA-N
Formula:	C13H22
SMILES:	CCC12CC3CC(CC(C)(C3)C1)C2
Mol. weight [g/mol]:	178.31
CAS:	1687-34-9

Physical Properties

Property code	Value	Unit	Source
gf	210.04	kJ/mol	Joback Method
hf	-89.27	kJ/mol	Joback Method
hfus	10.21	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	4.003		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1273.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	517.14	K	Joback Method
tc	739.37	K	Joback Method
tf	330.13	K	Joback Method
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.54	J/mol×K	517.14	Joback Method

cpg	440.16	J/mol×K	554.18	Joback Method
cpg	460.91	J/mol×K	591.22	Joback Method
cpg	480.10	J/mol×K	628.26	Joback Method
cpg	498.02	J/mol×K	665.29	Joback Method
cpg	514.97	J/mol×K	702.33	Joback Method
cpg	531.25	J/mol×K	739.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1687349&Units=SI
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

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

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