

3,5,7-trimethyl-1-adamantanol

Inchi:	InChI=1S/C13H22O/c1-10-4-11(2)6-12(3,5-10)9-13(14,7-10)8-11/h14H,4-9H2,1-3H3
InchiKey:	DVKFVAJDHKVYLK-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	CC12CC3(C)CC(C)(C1)CC(O)(C2)C3
Mol. weight [g/mol]:	194.31

Physical Properties

Property code	Value	Unit	Source
gf	62.24	kJ/mol	Joback Method
hf	-211.02	kJ/mol	Joback Method
hfus	1.70	kJ/mol	Joback Method
hvap	56.21	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.118		Crippen Method
mcvol	167.320	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1304.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1304.00		NIST Webbook
ripol	1785.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1785.00		NIST Webbook
tb	609.80	K	Joback Method
tc	831.80	K	Joback Method
tf	438.75	K	Joback Method
vc	0.636	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.73	J/mol×K	609.80	Joback Method

cpg	499.70	J/mol×K	646.80	Joback Method
cpg	515.77	J/mol×K	683.80	Joback Method
cpg	531.43	J/mol×K	720.80	Joback Method
cpg	547.16	J/mol×K	757.80	Joback Method
cpg	563.43	J/mol×K	794.80	Joback Method
cpg	580.73	J/mol×K	831.80	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=R304655&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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