

3-isopropyl-1-adamantanol

Inchi:	InChI=1S/C13H22O/c1-9(2)12-4-10-3-11(5-12)7-13(14,6-10)8-12/h9-11,14H,3-8H2,1-2H
InchiKey:	CIGVNBDLKNGATQ-UHFFFAOYSA-N
Formula:	C13H22O
SMILES:	CC(C)C12CC3CC(CC(O)(C3)C1)C2
Mol. weight [g/mol]:	194.31

Physical Properties

Property code	Value	Unit	Source
gf	70.78	kJ/mol	Joback Method
hf	-246.78	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.974		Crippen Method
mcvol	167.320	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1506.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2122.00		NIST Webbook
tb	608.88	K	Joback Method
tc	819.09	K	Joback Method
tf	375.95	K	Joback Method
vc	0.634	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.78	J/mol×K	608.88	Joback Method
cpg	505.66	J/mol×K	643.91	Joback Method
cpg	522.48	J/mol×K	678.95	Joback Method

cpg	538.50	J/mol×K	713.98	Joback Method
cpg	553.97	J/mol×K	749.02	Joback Method
cpg	569.15	J/mol×K	784.05	Joback Method
cpg	584.28	J/mol×K	819.09	Joback Method

Sources

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=R304739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	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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