

3-(1-adamantyl)pentane

Other names:	1-(1-Ethylpropyl)adamantane
Inchi:	InChI=1S/C15H26/c1-3-14(4-2)15-8-11-5-12(9-15)7-13(6-11)10-15/h11-14H,3-10H2,1-2H
InchiKey:	QHRWEUGZPFJFJT-VKXBSSMUSA-N
Formula:	C15H26
SMILES:	CCC(CC)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	229.93	kJ/mol	Joback Method
hf	-151.07	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.639		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1568.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1539.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1767.00		NIST Webbook
ripol	1744.00		NIST Webbook
tb	562.22	K	Joback Method
tc	773.10	K	Joback Method
tf	313.77	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	521.46	J/mol×K	562.22	Joback Method
cpg	544.87	J/mol×K	597.37	Joback Method
cpg	566.74	J/mol×K	632.51	Joback Method
cpg	587.25	J/mol×K	667.66	Joback Method
cpg	606.59	J/mol×K	702.81	Joback Method
cpg	624.94	J/mol×K	737.96	Joback Method
cpg	642.48	J/mol×K	773.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R134540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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