

2-isobutylideneadamantane

Inchi:	InChI=1S/C14H22/c1-9(2)3-14-12-5-10-4-11(7-12)8-13(14)6-10/h3,9-13H,4-8H2,1-2H3/b
InchiKey:	AJPQLQKXRCBRCK-BNNQUZSASA-N
Formula:	C14H22
SMILES:	CC(C)C=C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	272.46	kJ/mol	Joback Method
hf	-69.64	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	46.76	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.025		Crippen Method
mcvol	171.240	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1402.00		NIST Webbook
rinpol	1370.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1391.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1534.00		NIST Webbook
tb	545.74	K	Joback Method
tc	758.47	K	Joback Method
tf	288.96	K	Joback Method
vc	0.658	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.44	J/mol×K	545.74	Joback Method
cpg	474.65	J/mol×K	581.20	Joback Method
cpg	495.41	J/mol×K	616.65	Joback Method

cpg	514.82	J/molxK	652.11	Joback Method
cpg	532.98	J/molxK	687.56	Joback Method
cpg	550.01	J/molxK	723.02	Joback Method
cpg	566.01	J/molxK	758.47	Joback Method
dvisc	0.0013449	Paxs	288.96	Joback Method
dvisc	0.0013608	Paxs	331.76	Joback Method
dvisc	0.0013732	Paxs	374.55	Joback Method
dvisc	0.0013831	Paxs	417.35	Joback Method
dvisc	0.0013913	Paxs	460.15	Joback Method
dvisc	0.0013981	Paxs	502.94	Joback Method
dvisc	0.0014038	Paxs	545.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304571&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
dvisc:	Dynamic viscosity
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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