2-isobutyladamantane

Inchi: InChI=1S/C14H24/c1-9(2)3-14-12-5-10-4-11(7-12)8-13(14)6-10/h9-14H,3-8H2,1-2H3/t10
InchiKey: MEVUXHARANYDNT-PWHQIARISA-N
Formula: C14H24
SMILES: CC(C)CC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 192.34

Physical Properties

Property code	Value	Unit	Source
gf	219.29	kJ/mol	Joback Method
hf	-166.01	kJ/mol	Joback Method
hfus	22.94	kJ/mol	Joback Method
hvap	45.66	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	4.105		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1423.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1581.00		NIST Webbook
tb	534.43	K	Joback Method
tc	740.27	K	Joback Method
tf	274.36	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.51	J/mol×K	534.43	Joback Method
cpg	493.24	J/mol×K	568.74	Joback Method
cpg	515.51	J/mol×K	603.04	Joback Method
cpg	536.42	J/mol×K	637.35	Joback Method
cpg	556.04	J/mol×K	671.65	Joback Method
cpg	574.47	J/mol×K	705.96	Joback Method
cpg	591.80	J/mol×K	740.27	Joback Method
dvisc	0.0012042	Pa×s	274.36	Joback Method
dvisc	0.0013059	Pa×s	317.70	Joback Method
dvisc	0.0013889	Pa×s	361.05	Joback Method
dvisc	0.0014578	Pa×s	404.39	Joback Method
dvisc	0.0015158	Pa×s	447.74	Joback Method
dvisc	0.0015653	Pa×s	491.08	Joback Method
dvisc	0.0016080	Pa×s	534.43	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R134500&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
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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