1-isopropyladamantane

Inchi: InChI=1S/C13H22/c1-9(2)13-6-10-3-11(7-13)5-12(4-10)8-13/h9-12H,3-8H2,1-2H3/t10-,11
InchiKey: ISDSLPMQFWIUPU-XYIZDEMUSA-N
Formula: C13H22
SMILES: CC(C)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 178.31

Physical Properties

Property code	Value	Unit	Source
gf	213.09	kJ/mol	Joback Method
hf	-109.79	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	42.59	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.859		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1358.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1583.00		NIST Webbook
tb	516.46	K	Joback Method

tc	734.47	K	Joback Method
tf	291.23	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.80	J/mol×K	516.46	Joback Method
cpg	440.91	J/mol×K	552.80	Joback Method
cpg	462.31	J/mol×K	589.13	Joback Method
cpg	482.19	J/mol×K	625.47	Joback Method
cpg	500.75	J/mol×K	661.80	Joback Method
cpg	518.19	J/mol×K	698.14	Joback Method
cpg	534.69	J/mol×K	734.47	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R134446&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
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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