1-propyladamantane

Other names: 1-n-propyl-adamantane
Inchi: InChI=1S/C13H22/c1-2-3-13-7-10-4-11(8-13)6-12(5-10)9-13/h10-12H,2-9H2,1H3/t10-,11
InchiKey: SCKYQTNMKBTHDQ-XYIZDEMUSA-N
Formula: C13H22
SMILES: CCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 178.31

Physical Properties

Property code	Value	Unit	Source
gf	215.53	kJ/mol	Joback Method
hf	-104.51	kJ/mol	Joback Method
hfus	16.50	kJ/mol	Joback Method
hvap	42.98	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	4.003		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1346.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1373.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1552.00		NIST Webbook
tb	516.90	K	Joback Method
tc	730.05	K	Joback Method
tf	306.23	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.63	J/mol×K	516.90	Joback Method
cpg	440.16	J/mol×K	552.42	Joback Method
cpg	461.05	J/mol×K	587.95	Joback Method
cpg	480.49	J/mol×K	623.47	Joback Method
cpg	498.67	J/mol×K	659.00	Joback Method
cpg	515.78	J/mol×K	694.52	Joback Method
cpg	531.98	J/mol×K	730.05	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R134451&Units=SI

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