2-n-Propyladamantane

Other names: 2-Propyladamantane
Inchi: InChI=1S/C13H22/c1-2-3-13-11-5-9-4-10(7-11)8-12(13)6-9/h9-13H,2-8H2,1H3
InchiKey: HMUYSRNQYPLWHB-UHFFFAOYSA-N
Formula: C13H22
SMILES: CCCC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 178.31
CAS: 14451-88-8

Physical Properties

Property code	Value	Unit	Source
gf	213.31	kJ/mol	Joback Method
hf	-140.09	kJ/mol	Joback Method
hfus	23.87	kJ/mol	Joback Method
hvap	43.83	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.859		Crippen Method
mcvol	161.450	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1363.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1559.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1601.00		NIST Webbook
tb	511.99	K	Joback Method

tc	716.41	K	Joback Method
tf	278.09	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.65	J/mol×K	511.99	Joback Method
cpg	440.53	J/mol×K	546.06	Joback Method
cpg	462.00	J/mol×K	580.13	Joback Method
cpg	482.15	J/mol×K	614.20	Joback Method
cpg	501.07	J/mol×K	648.27	Joback Method
cpg	518.83	J/mol×K	682.34	Joback Method
cpg	535.53	J/mol×K	716.41	Joback Method
dvisc	0.0009768	Pa×s	278.09	Joback Method
dvisc	0.0011128	Pa×s	317.07	Joback Method
dvisc	0.0012322	Pa×s	356.06	Joback Method
dvisc	0.0013372	Pa×s	395.04	Joback Method
dvisc	0.0014299	Pa×s	434.02	Joback Method
dvisc	0.0015123	Pa×s	473.01	Joback Method
dvisc	0.0015859	Pa×s	511.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14451888&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