2-propylideneadamantane

Inchi: InChI=1S/C13H20/c1-2-3-13-11-5-9-4-10(7-11)8-12(13)6-9/h3,9-12H,2,4-8H2,1H3/b13-3
InchiKey: NMSHDLHOYYNLED-DXNYSGJVSA-N
Formula: C13H20
SMILES: CCC=C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	266.48	kJ/mol	Joback Method
hf	-43.72	kJ/mol	Joback Method
hfus	23.13	kJ/mol	Joback Method
hvap	44.92	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.779		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1339.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1339.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	523.30	K	Joback Method
tc	734.81	K	Joback Method
tf	292.69	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.50	J/mol×K	523.30	Joback Method
cpg	422.85	J/mol×K	558.55	Joback Method

cpg	442.78	J/mol×K	593.80	Joback Method
cpg	461.41	J/mol×K	629.06	Joback Method
cpg	478.83	J/mol×K	664.31	Joback Method
cpg	495.15	J/mol×K	699.56	Joback Method
cpg	510.46	J/mol×K	734.81	Joback Method
dvisc	0.0011085	Pa×s	292.69	Joback Method
dvisc	0.0011803	Pa×s	331.12	Joback Method
dvisc	0.0012405	Pa×s	369.56	Joback Method
dvisc	0.0012916	Pa×s	408.00	Joback Method
dvisc	0.0013355	Pa×s	446.43	Joback Method
dvisc	0.0013735	Pa×s	484.87	Joback Method
dvisc	0.0014069	Pa×s	523.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304635&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