2-isopropylideneadamantane

Inchi: InChI=1S/C13H20/c1-8(2)13-11-4-9-3-10(6-11)7-12(13)5-9/h9-12H,3-7H2,1-2H3
InchiKey: WMXHJGRQXBTIFH-UHFFFAOYSA-N
Formula: C13H20
SMILES: CC(C)=C1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	257.93	kJ/mol	Joback Method
hf	-53.51	kJ/mol	Joback Method
hfus	21.82	kJ/mol	Joback Method
hvap	45.00	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.779		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1359.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1554.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1554.00		NIST Webbook
tb	523.18	K	Joback Method
tc	738.71	K	Joback Method
tf	278.73	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.32	J/mol×K	523.18	Joback Method
cpg	423.03	J/mol×K	559.10	Joback Method

cpg	443.27	J/mol×K	595.02	Joback Method
cpg	462.17	J/mol×K	630.94	Joback Method
cpg	479.82	J/mol×K	666.87	Joback Method
cpg	496.33	J/mol×K	702.79	Joback Method
cpg	511.81	J/mol×K	738.71	Joback Method

Sources

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=R304586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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