2-(1-adamantyl)propene

Inchi: InChI=1S/C13H20/c1-9(2)13-6-10-3-11(7-13)5-12(4-10)8-13/h10-12H,1,3-8H2,2H3
InchiKey: IATJIZFUHGLZBF-UHFFFAOYSA-N
Formula: C13H20
SMILES: C=C(C)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	294.82	kJ/mol	Joback Method
hf	11.13	kJ/mol	Joback Method
hfus	13.91	kJ/mol	Joback Method
hvap	42.39	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.779		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1374.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1643.00		NIST Webbook
ripol	1618.00		NIST Webbook
tb	513.46	K	Joback Method
tc	735.56	K	Joback Method
tf	290.51	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.31	J/mol×K	513.46	Joback Method
cpg	420.78	J/mol×K	550.48	Joback Method

cpg	441.49	J/mol×K	587.49	Joback Method
cpg	460.65	J/mol×K	624.51	Joback Method
cpg	478.48	J/mol×K	661.52	Joback Method
cpg	495.18	J/mol×K	698.54	Joback Method
cpg	510.97	J/mol×K	735.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304506&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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