4-ethylidene-2-thiaadamantane

Inchi: InChI=1S/C11H16S/c1-2-10-8-3-7-4-9(6-8)12-11(10)5-7/h2,7-9,11H,3-6H2,1H3/b10-2+
InchiKey: OGNJHZQCNYTMRS-WTDSWWLTSA-N
Formula: C11H16S
SMILES: CC=C1C2CC3CC(C2)SC1C3
Mol. weight [g/mol]: 180.31

Physical Properties

Property code	Value	Unit	Source
gf	289.50	kJ/mol	Joback Method
hf	42.82	kJ/mol	Joback Method
hfus	21.60	kJ/mol	Joback Method
hvap	46.28	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.237		Crippen Method
mcvol	145.320	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1563.00		NIST Webbook
tb	525.37	K	Joback Method
tc	757.07	K	Joback Method
tf	353.60	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.88	J/mol×K	525.37	Joback Method
cpg	376.59	J/mol×K	563.99	Joback Method
cpg	394.81	J/mol×K	602.60	Joback Method
cpg	411.69	J/mol×K	641.22	Joback Method

cpg	427.34	J/mol×K	679.83	Joback Method
cpg	441.90	J/mol×K	718.45	Joback Method
cpg	455.49	J/mol×K	757.07	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=R208032&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume