4-methylene-2-thiaadamantane

Inchi: InChI=1S/C10H14S/c1-6-8-2-7-3-9(5-8)11-10(6)4-7/h7-10H,1-5H2
InchiKey: YBMSHDNMHSMINO-UHFFFAOYSA-N
Formula: C10H14S
SMILES: C=C1C2CC3CC(C2)SC1C3
Mol. weight [g/mol]: 166.28

Physical Properties

Property code	Value	Unit	Source
gf	288.70	kJ/mol	Joback Method
hf	71.67	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	43.43	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.847		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1462.00		NIST Webbook
tb	495.01	K	Joback Method
tc	725.07	K	Joback Method
tf	345.65	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.70	J/mol×K	495.01	Joback Method
cpg	327.61	J/mol×K	533.35	Joback Method
cpg	345.10	J/mol×K	571.70	Joback Method
cpg	361.29	J/mol×K	610.04	Joback Method
cpg	376.29	J/mol×K	648.39	Joback Method
cpg	390.20	J/mol×K	686.73	Joback Method

cpg	403.14	J/mol×K	725.07	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=R208052&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