4,8-dimethylene-2-thiaadamantane

Inchi: InChI=1S/C11H14S/c1-6-8-3-9-5-10(6)12-11(4-8)7(9)2/h8-11H,1-5H2
InchiKey: YTWVHGATJGAWAV-UHFFFAOYSA-N
Formula: C11H14S
SMILES: C=C1C2CC3CC1SC(C2)C3=C
Mol. weight [g/mol]: 178.29

Physical Properties

Property code	Value	Unit	Source
gf	350.20	kJ/mol	Joback Method
hf	135.27	kJ/mol	Joback Method
hfus	18.96	kJ/mol	Joback Method
hvap	45.81	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.013		Crippen Method
mcvol	141.020	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1498.00		NIST Webbook
tb	517.05	K	Joback Method
tc	745.15	K	Joback Method
tf	370.60	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.28	J/mol×K	517.05	Joback Method
cpg	355.34	J/mol×K	555.07	Joback Method
cpg	372.10	J/mol×K	593.08	Joback Method
cpg	387.66	J/mol×K	631.10	Joback Method
cpg	402.12	J/mol×K	669.12	Joback Method
cpg	415.59	J/mol×K	707.13	Joback Method

cpg	428.16	J/mol×K	745.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R208047&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

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