2-Thiaadamantan-4-ol

Inchi: InChI=1S/C9H14OS/c10-9-6-1-5-2-7(4-6)11-8(9)3-5/h5-10H,1-4H2
InchiKey: QYWXGQGTCFPNAY-UHFFFAOYSA-N
Formula: C9H14OS
SMILES: OC1C2CC3CC(C2)SC1C3
Mol. weight [g/mol]: 170.27
CAS: 40801-15-8

Physical Properties

Property code	Value	Unit	Source
gf	82.67	kJ/mol	Joback Method
hf	-164.50	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.651		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	1222.00		NIST Webbook
rinpol	1222.00		NIST Webbook
tb	560.48	K	Joback Method
tc	774.70	K	Joback Method
tf	377.28	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.50	J/mol×K	560.48	Joback Method
cpg	358.45	J/mol×K	596.18	Joback Method
cpg	373.29	J/mol×K	631.89	Joback Method
cpg	387.11	J/mol×K	667.59	Joback Method
cpg	400.01	J/mol×K	703.30	Joback Method
cpg	412.06	J/mol×K	739.00	Joback Method
cpg	423.35	J/mol×K	774.70	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=C40801158&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