2-Thiatricyclo[3.3.1.1(3,7)]decane

Other names: 2-Thiaadamantane
Inchi: InChI=1S/C9H14S/c1-6-2-8-4-7(1)5-9(3-6)10-8/h6-9H,1-5H2
InchiKey: NOBCRSKNBOQNEL-UHFFFAOYSA-N
Formula: C9H14S
SMILES: C1C2CC3CC1CC(C2)S3
Mol. weight [g/mol]: 154.27
CAS: 281-25-4

Physical Properties

Property code	Value	Unit	Source
chs	-6000.86 ± 0.96	kJ/mol	NIST Webbook
gf	227.20	kJ/mol	Joback Method
hf	8.07	kJ/mol	Joback Method
hfs	-143.50 ± 1.10	kJ/mol	NIST Webbook
hfus	16.10	kJ/mol	Joback Method
hvap	41.04	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.680		Crippen Method
mcvol	121.440	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1449.00		NIST Webbook
tb	472.97	K	Joback Method
tc	704.84	K	Joback Method
tf	597.00 ± 3.00	K	NIST Webbook
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.72	J/mol×K	472.97	Joback Method
cpg	299.56	J/mol×K	511.61	Joback Method
cpg	317.85	J/mol×K	550.26	Joback Method

cpg	334.73	J/mol×K	588.90	Joback Method
cpg	350.31	J/mol×K	627.55	Joback Method
cpg	364.71	J/mol×K	666.19	Joback Method
cpg	378.05	J/mol×K	704.84	Joback Method
cps	213.00	J/mol×K	298.15	NIST Webbook
hfust	8.10	kJ/mol	597.00	NIST Webbook

Sources

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=C281254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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