Thiosulfuric acid, s-2-piperidylmethyl ester

Inchi: InChI=1S/C6H13NO3S2/c8-12(9,10)11-5-6-3-1-2-4-7-6/h6-7H,1-5H2,(H,8,9,10)
InchiKey: IEMJBVVWJLQAOK-UHFFFAOYSA-N
Formula: C6H13NO3S2
SMILES: O=S(=O)(O)SCC1CCCCN1
Mol. weight [g/mol]: 211.30
CAS: 1822-62-4

Physical Properties

Property code	Value	Unit	Source
gf	-460.44	kJ/mol	Joback Method
hf	-638.75	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	78.27	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	0.665		Crippen Method
mcvol	144.830	ml/mol	McGowan Method
pc	5917.16	kPa	Joback Method
tb	613.52	K	Joback Method
tc	825.87	K	Joback Method
tf	403.57	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.25	J/mol×K	613.52	Joback Method
cpg	373.67	J/mol×K	648.91	Joback Method
cpg	386.26	J/mol×K	684.30	Joback Method
cpg	397.99	J/mol×K	719.70	Joback Method
cpg	408.87	J/mol×K	755.09	Joback Method
cpg	418.88	J/mol×K	790.48	Joback Method
cpg	428.01	J/mol×K	825.87	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=C1822624&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume