Thiopropanal sulfoxide

Other names: Thiopropanal S-oxide
Inchi: InChI=1S/C3H6OS/c1-2-3-5-4/h3H,2H2,1H3
InchiKey: BAZSXBOAXJLRNH-UHFFFAOYSA-N
Formula: C3H6OS
SMILES: CCC=S=O
Mol. weight [g/mol]: 90.14

Physical Properties

Property code	Value	Unit	Source
gf	-150.84	kJ/mol	Joback Method
hf	-196.57	kJ/mol	Joback Method
hfus	13.06	kJ/mol	Joback Method
hvap	34.83	kJ/mol	Joback Method
log10ws	-0.19		Crippen Method
logp	0.412		Crippen Method
mcvol	71.050	ml/mol	McGowan Method
pc	5486.97	kPa	Joback Method
rinpol	740.00		NIST Webbook
rinpol	760.00		NIST Webbook
tb	327.70	K	Joback Method
tc	505.41	K	Joback Method
tf	173.88	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.23	J/mol×K	327.70	Joback Method
cpg	109.90	J/mol×K	357.32	Joback Method
cpg	116.19	J/mol×K	386.94	Joback Method
cpg	122.12	J/mol×K	416.56	Joback Method
cpg	127.70	J/mol×K	446.18	Joback Method
cpg	132.95	J/mol×K	475.80	Joback Method
cpg	137.89	J/mol×K	505.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322284&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