S-Propylmethanethiosulfonate

Other names: propyl methanethiosulfonate
Inchi: InChI=1S/C4H10O2S2/c1-3-4-7-8(2,5)6/h3-4H2,1-2H3
InchiKey: NTHJPLSCKRFMSP-UHFFFAOYSA-N
Formula: C4H10O2S2
SMILES: CCCSS(C)(=O)=O
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-452.62	kJ/mol	Joback Method
hf	-537.37	kJ/mol	Joback Method
hfus	21.62	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.089		Crippen Method
mcvol	111.660	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	1175.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1156.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	407.48	K	Joback Method
tc	595.52	K	Joback Method
tf	207.80	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.61	J/mol×K	407.48	Joback Method
cpg	211.26	J/mol×K	438.82	Joback Method
cpg	220.61	J/mol×K	470.16	Joback Method
cpg	229.63	J/mol×K	501.50	Joback Method
cpg	238.31	J/mol×K	532.84	Joback Method

cpg	246.65	J/mol×K	564.18	Joback Method
cpg	254.64	J/mol×K	595.52	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=U322287&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