S-Propylpropanethiosulfonate

Other names: dipropyl thiosulfonate
Propyl propanethiosulfonate
Inchi: InChI=1S/C6H14O2S2/c1-3-5-9-10(7,8)6-4-2/h3-6H2,1-2H3
InchiKey: OUIASSQOLAEHIR-UHFFFAOYSA-N
Formula: C6H14O2S2
SMILES: CCCSS(=O)(=O)CCC
Mol. weight [g/mol]: 182.30

Physical Properties

Property code	Value	Unit	Source
gf	-435.78	kJ/mol	Joback Method
hf	-578.65	kJ/mol	Joback Method
hfus	26.80	kJ/mol	Joback Method
hvap	54.40	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.869		Crippen Method
mcvol	139.840	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1348.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1348.00		NIST Webbook
ripol	2124.00		NIST Webbook
tb	453.24	K	Joback Method
tc	638.07	K	Joback Method
tf	230.34	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.77	J/mol×K	453.24	Joback Method
cpg	292.00	J/mol×K	484.04	Joback Method
cpg	303.78	J/mol×K	514.85	Joback Method

cpg	315.09	J/mol×K	545.65	Joback Method
cpg	325.94	J/mol×K	576.46	Joback Method
cpg	336.31	J/mol×K	607.26	Joback Method
cpg	346.20	J/mol×K	638.07	Joback Method

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=U322291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume