Ethyl 1-(methylthio)propyl disulphide

Inchi: InChI=1S/C6H14S3/c1-4-6(7-3)9-8-5-2/h6H,4-5H2,1-3H3
InchiKey: YPJBMNWGGROJKJ-UHFFFAOYSA-N
Formula: C6H14S3
SMILES: CCSSC(CC)SC
Mol. weight [g/mol]: 182.37

Physical Properties

Property code	Value	Unit	Source
gf	96.56	kJ/mol	Joback Method
hf	-46.84	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	49.01	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.487		Crippen Method
mcvol	144.450	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
tb	542.58	K	Joback Method
tc	781.71	K	Joback Method
tf	245.58	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.78	J/mol×K	542.58	Joback Method
cpg	315.03	J/mol×K	582.43	Joback Method
cpg	327.57	J/mol×K	622.29	Joback Method
cpg	339.39	J/mol×K	662.14	Joback Method
cpg	350.47	J/mol×K	702.00	Joback Method
cpg	360.81	J/mol×K	741.85	Joback Method
cpg	370.39	J/mol×K	781.71	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=R226070&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