Ethyl(methylthio)methyl disulphide

Inchi: InChI=1S/C4H10S3/c1-3-6-7-4-5-2/h3-4H2,1-2H3
InchiKey: LGRRPFGGSKUKDE-UHFFFAOYSA-N
Formula: C4H10S3
SMILES: CCSSCSC
Mol. weight [g/mol]: 154.32

Physical Properties

Property code	Value	Unit	Source
gf	82.16	kJ/mol	Joback Method
hf	-0.28	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.708		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
ripol	1716.20		NIST Webbook
ripol	1716.20		NIST Webbook
tb	497.26	K	Joback Method
tc	740.19	K	Joback Method
tf	238.04	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.75	J/mol×K	497.26	Joback Method
cpg	227.03	J/mol×K	537.75	Joback Method
cpg	236.83	J/mol×K	578.24	Joback Method
cpg	246.12	J/mol×K	618.73	Joback Method
cpg	254.89	J/mol×K	659.22	Joback Method
cpg	263.12	J/mol×K	699.70	Joback Method
cpg	270.79	J/mol×K	740.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R327589&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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