Methyl 1-(methylthio)ethyl disulphide

Other names: Methyl 1-(methylthio)ethyl disulphide
1-(Methylthioethyl) methyl disulfide
Inchi: InChI=1S/C4H10S3/c1-4(5-2)7-6-3/h4H,1-3H3
InchiKey: BILDZELNIVRXQA-UHFFFAOYSA-N
Formula: C4H10S3
SMILES: CSSC(C)SC
Mol. weight [g/mol]: 154.33

Physical Properties

Property code	Value	Unit	Source
af	0.2678		Cheméo Relay (1.0)
hf	-37.24	kJ/mol	Cheméo Relay (1.0)
hfus	14.98	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Cheméo Relay (1.0)
ie	8.39	eV	Cheméo Relay (1.0)
logp	2.707		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1144.00		NIST Webbook
tb	479.69	K	Cheméo Relay (1.0)
tc	688.85	K	Cheméo Relay (1.0)
tf	222.05	K	Cheméo Relay (1.0)
vc	0.390	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.04	J/mol×K	496.82	Joback Method
cpg	227.67	J/mol×K	538.31	Joback Method
cpg	237.77	J/mol×K	579.80	Joback Method
cpg	247.33	J/mol×K	621.29	Joback Method
cpg	256.33	J/mol×K	662.79	Joback Method
cpg	264.74	J/mol×K	704.28	Joback Method
cpg	272.55	J/mol×K	745.77	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4413290&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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