4-methyl-2,3,5-trithiahexane

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]: 154.32
CAS: 4413-29-0

Physical Properties

Property code	Value	Unit	Source
gf	79.72	kJ/mol	Joback Method
hf	-5.56	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	44.56	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.707		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpol	1131.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1145.00		NIST Webbook
tb	496.82	K	Joback Method
tc	745.77	K	Joback Method
tf	223.04	K	Joback Method
vc	0.415	m3/kmol	Joback Method

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

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=C4413290&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