1-(methylthio)ethanethiol

Other names: 3-Thia-2-butanethiol
1-Ethanethiol, 1-(methylthio)
Ethanethiol, 1-methylthio
Inchi: InChI=1S/C3H8S2/c1-3(4)5-2/h3-4H,1-2H3
InchiKey: GHIADNFHCKUPJL-UHFFFAOYSA-N
Formula: C3H8S2
SMILES: CSC(C)S
Mol. weight [g/mol]: 108.23

Physical Properties

Property code	Value	Unit	Source
gf	34.45	kJ/mol	Joback Method
hf	-30.18	kJ/mol	Joback Method
hfus	8.17	kJ/mol	Joback Method
hvap	35.44	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.625		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	4980.35	kPa	Joback Method
rinpol	826.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	861.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	826.00		NIST Webbook
rinpol	861.00		NIST Webbook
tb	399.24	K	Joback Method
tc	625.81	K	Joback Method
tf	179.43	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.54	J/mol×K	399.24	Joback Method
cpg	147.58	J/mol×K	437.00	Joback Method
cpg	155.28	J/mol×K	474.76	Joback Method
cpg	162.63	J/mol×K	512.52	Joback Method
cpg	169.64	J/mol×K	550.28	Joback Method
cpg	176.30	J/mol×K	588.04	Joback Method
cpg	182.61	J/mol×K	625.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R61045&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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