Methanedithiol

Other names:	dithiomethane
	Dimercaptomethane
Inchi:	InChI=1S/CH4S2/c2-1-3/h2-3H,1H2
InchiKey:	INBDPOJZYZJUDA-UHFFFAOYSA-N
Formula:	CH4S2
SMILES:	SCS
Mol. weight [g/mol]:	80.17
CAS:	6725-64-0

Physical Properties

Property code	Value	Unit	Source
gf	16.32	kJ/mol	Joback Method
hf	12.99	kJ/mol	Joback Method
hfus	6.43	kJ/mol	Joback Method
hvap	31.29	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
log10ws	-0.88		Crippen Method
logp	0.803		Crippen Method
mcvol	57.650	ml/mol	McGowan Method
pc	7109.36	kPa	Joback Method
rinpol	692.00		NIST Webbook
rinpol	740.00		NIST Webbook
rinpol	661.00		NIST Webbook
rinpol	661.00		NIST Webbook
tb	348.00	K	Joback Method
tc	572.75	K	Joback Method
tf	173.95	K	Joback Method
vc	0.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.51	J/mol×K	348.00	Joback Method
cpg	80.37	J/mol×K	385.46	Joback Method

cpg	84.05	J/mol×K	422.92	Joback Method
cpg	87.56	J/mol×K	460.38	Joback Method
cpg	90.91	J/mol×K	497.84	Joback Method
cpg	94.10	J/mol×K	535.29	Joback Method
cpg	97.12	J/mol×K	572.75	Joback Method

Sources

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=C6725640&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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