Methyl hydrogen disulfide

Other names:	Methyl hydrodisulfide
	Methyl sulfhydryl sulfide
	Hydrogen methyl disulfide
Inchi:	InChI=1S/CH4S2/c1-3-2/h2H,1H3
InchiKey:	KFLNNVFDKSNGBW-UHFFFAOYSA-N
Formula:	CH4S2
SMILES:	CSS
Mol. weight [g/mol]:	80.17
CAS:	6251-26-9

Physical Properties

Property code	Value	Unit	Source
gf	20.05	kJ/mol	Joback Method
hf	16.38	kJ/mol	Joback Method
hfus	6.52	kJ/mol	Joback Method
hvap	31.37	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.194		Crippen Method
mcvol	57.650	ml/mol	McGowan Method
pc	6577.70	kPa	Joback Method
rinpol	686.00		NIST Webbook
rinpol	640.00		NIST Webbook
rinpol	686.00		NIST Webbook
tb	353.92	K	Joback Method
tc	579.02	K	Joback Method
tf	171.89	K	Joback Method
vc	0.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	76.57	J/mol×K	353.92	Joback Method
cpg	80.40	J/mol×K	391.44	Joback Method
cpg	84.13	J/mol×K	428.95	Joback Method

cpg	87.74	J/mol×K	466.47	Joback Method
cpg	91.23	J/mol×K	503.99	Joback Method
cpg	94.59	J/mol×K	541.51	Joback Method
cpg	97.82	J/mol×K	579.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6251269&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

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