Mercaptomethyl radical

Inchi: InChI=1S/CH3S/c1-2/h2H,1H2
InchiKey: YYOGAOHWUDJBLM-UHFFFAOYSA-N
Formula: CH3S
SMILES: [CH2]S
Mol. weight [g/mol]: 47.10
CAS: 17032-46-1

Physical Properties

Property code	Value	Unit	Source
affp	733.90	kJ/mol	NIST Webbook
basg	701.50	kJ/mol	NIST Webbook
ea	0.78 ± 0.33	eV	NIST Webbook
gf	39.31	kJ/mol	Joback Method
hf	30.32	kJ/mol	Joback Method
hfus	4.07	kJ/mol	Joback Method
hvap	24.41	kJ/mol	Joback Method
ie	7.54 ± 0.00	eV	NIST Webbook
log10ws	-0.42		Crippen Method
logp	0.708		Crippen Method
mcvol	39.150	ml/mol	McGowan Method
pc	6875.52	kPa	Joback Method
tb	284.44	K	Joback Method
tc	470.35	K	Joback Method
tf	153.86	K	Joback Method
vc	0.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	43.23	J/mol×K	284.44	Joback Method
cpg	46.45	J/mol×K	315.42	Joback Method
cpg	49.39	J/mol×K	346.41	Joback Method
cpg	52.05	J/mol×K	377.39	Joback Method
cpg	54.46	J/mol×K	408.38	Joback Method

cpg	56.64	J/mol×K	439.36	Joback Method
cpg	58.61	J/mol×K	470.35	Joback Method

Sources

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=C17032461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume