

MeS anion

Inchi:	InChI=1S/CH4S/c1-2/h2H,1H3/p-1
InchiKey:	LSDPWZHWYPCBBB-UHFFFAOYSA-M
Formula:	CH3S-
SMILES:	C[S-]
Mol. weight [g/mol]:	47.10
CAS:	17302-63-5

Physical Properties

Property code	Value	Unit	Source
gf	43.04	kJ/mol	Joback Method
hf	33.71	kJ/mol	Joback Method
hfus	4.16	kJ/mol	Joback Method
hvap	24.49	kJ/mol	Joback Method
log10ws	0.88		Crippen Method
logp	0.163		Crippen Method
mcvol	39.150	ml/mol	McGowan Method
pc	6369.39	kPa	Joback Method
tb	290.36	K	Joback Method
tc	477.24	K	Joback Method
tf	151.80	K	Joback Method
vc	0.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	43.49	J/molxK	290.36	Joback Method
cpg	46.55	J/molxK	321.51	Joback Method
cpg	49.38	J/molxK	352.65	Joback Method
cpg	52.00	J/molxK	383.80	Joback Method
cpg	54.41	J/molxK	414.95	Joback Method
cpg	56.63	J/molxK	446.09	Joback Method
cpg	58.69	J/molxK	477.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17302635&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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