Methane-d3,(methylthio)

Inchi: InChI=1S/C2H6S/c1-3-2/h1-2H3/i1D3
InchiKey: QMMFVYPAHWMCMS-FIBGUPNXSA-N
Formula: C2H3D3S
SMILES: CSC
Mol. weight [g/mol]: 65.15
CAS: 4752-12-9

Physical Properties

Property code	Value	Unit	Source
gf	-0.92	kJ/mol	Joback Method
hf	-42.74	kJ/mol	Joback Method
hfus	5.07	kJ/mol	Joback Method
hvap	26.86	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-0.54		Crippen Method
logp	0.979		Crippen Method
mcvol	55.390	ml/mol	McGowan Method
pc	5153.45	kPa	Joback Method
tb	313.94	K	Joback Method
tc	505.47	K	Joback Method
tf	146.70	K	Joback Method
vc	0.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.88	J/mol×K	313.94	Joback Method
cpg	79.79	J/mol×K	345.86	Joback Method
cpg	84.58	J/mol×K	377.78	Joback Method
cpg	89.24	J/mol×K	409.70	Joback Method
cpg	93.77	J/mol×K	441.62	Joback Method
cpg	98.17	J/mol×K	473.55	Joback Method
cpg	102.43	J/mol×K	505.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4752129&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
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