Ethanol, 2-(methylthio)-

Other names:	Hydroxyethyl methyl sulfide
	«beta»-Hydroxyethyl methyl sulfide
	2-Hydroxyethyl methyl sulfide
	Methyl 2-hydroxyethyl sulfide
	S-Methylmercaptoethanol
	«beta»-Methylmercaptoethanol
	2-Methylmercaptoethanol
	«beta»-(Methylthio)ethanol
	2-(Methylthio)ethanol
	1-Hydroxy-2-(methylthio)-ethane
	2-Methylthioethanol
	NSC 1902
Inchi:	InChI=1S/C3H8OS/c1-5-3-2-4/h4H,2-3H2,1H3
InchiKey:	WBBPRCNXBQTYLF-UHFFFAOYSA-N
Formula:	C3H8OS
SMILES:	CSCCO
Mol. weight [g/mol]:	92.16
CAS:	5271-38-5

Physical Properties

Property code	Value	Unit	Source
gf	-129.32	kJ/mol	Joback Method
hf	-215.61	kJ/mol	Joback Method
hfus	11.74	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-0.23		Crippen Method
logp	0.342		Crippen Method
mcvol	75.350	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
rinpol	810.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	844.00		NIST Webbook
rinpol	850.00		NIST Webbook
rinpol	813.00		NIST Webbook
ripol	1515.00		NIST Webbook

ripol	1497.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1533.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1526.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1502.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1534.00		NIST Webbook
ripol	1515.00		NIST Webbook
tb	443.20	K	NIST Webbook
tc	614.56	K	Joback Method
tf	218.79	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.81	J/mol×K	429.00	Joback Method
cpg	144.18	J/mol×K	459.93	Joback Method
cpg	150.32	J/mol×K	490.85	Joback Method
cpg	156.23	J/mol×K	521.78	Joback Method
cpg	161.92	J/mol×K	552.71	Joback Method
cpg	167.37	J/mol×K	583.64	Joback Method
cpg	172.60	J/mol×K	614.56	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5271385&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume