

Ethanol, 2-(ethylthio)-

Other names:	2-(Ethylthio)ethanol «beta»-Ethylthioethanol «beta»-Hydroxydiethyl sulfide Ethyl «beta»-hydroxyethyl sulfide Ethyl 2-hydroxyethyl sulfide Ethyl 2-hydroxyethyl thioether 2-Hydroxyethyl ethyl sulfide Ethyl thioethanol «beta»-ethylmerkptoethanol NSC 57105
Inchi:	InChI=1S/C4H10OS/c1-2-6-4-3-5/h5H,2-4H2,1H3
InchiKey:	LNRIEBFNWGMXKP-UHFFFAOYSA-N
Formula:	C4H10OS
SMILES:	CCSCCO
Mol. weight [g/mol]:	106.19
CAS:	110-77-0

Physical Properties

Property code	Value	Unit	Source
gf	-120.90	kJ/mol	Joback Method
hf	-236.25	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	47.99	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.732		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	455.20	K	NIST Webbook
tb	454.50 ± 1.50	K	NIST Webbook
tb	457.20	K	NIST Webbook
tc	635.80	K	Joback Method
tf	230.06	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.56	J/mol×K	451.88	Joback Method
cpg	182.30	J/mol×K	482.53	Joback Method
cpg	189.74	J/mol×K	513.19	Joback Method
cpg	196.89	J/mol×K	543.84	Joback Method
cpg	203.75	J/mol×K	574.49	Joback Method
cpg	210.33	J/mol×K	605.15	Joback Method
cpg	216.63	J/mol×K	635.80	Joback Method

Sources

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=C110770&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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