

2-Hydroxyethyl isopropyl sulfide

Other names:	Ethanol, 2-[(1-methylethyl)thio]- 2-[(1-methylethyl)thio]ethanol
Inchi:	InChI=1S/C5H12OS/c1-5(2)7-4-3-6/h5-6H,3-4H2,1-2H3
InchiKey:	QGONIKZRWOHHBB-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CC(C)SCCO
Mol. weight [g/mol]:	120.21
CAS:	40811-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-114.92	kJ/mol	Joback Method
hf	-262.17	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	49.83	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	1.120		Crippen Method
mvol	103.530	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	474.32	K	Joback Method
tc	660.48	K	Joback Method
tf	226.33	K	Joback Method
vc	0.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.79	J/molxK	474.32	Joback Method
cpg	223.03	J/molxK	505.35	Joback Method
cpg	231.90	J/molxK	536.37	Joback Method
cpg	240.40	J/molxK	567.40	Joback Method
cpg	248.53	J/molxK	598.42	Joback Method
cpg	256.30	J/molxK	629.45	Joback Method
cpg	263.71	J/molxK	660.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40811492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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