

2-Methanesulfonylethanol

Other names:	2-Hydroxyethylmethyl sulfone Ethanol, 2-(methylsulfonyl)- 2-(methylsulphonyl)ethanol
Inchi:	InChI=1S/C3H8O3S/c1-7(5,6)3-2-4/h4H,2-3H2,1H3
InchiKey:	KFTYFTKODBWKOU-UHFFFAOYSA-N
Formula:	C3H8O3S
SMILES:	CS(=O)(=O)CCO
Mol. weight [g/mol]:	124.16
CAS:	15205-66-0

Physical Properties

Property code	Value	Unit	Source
gf	-630.98	kJ/mol	Joback Method
hf	-710.83	kJ/mol	Joback Method
hfus	18.99	kJ/mol	Joback Method
hvap	57.59	kJ/mol	Joback Method
log10ws	0.82		Crippen Method
logp	-0.977		Crippen Method
mcvol	87.090	ml/mol	McGowan Method
pc	6308.83	kPa	Joback Method
tb	408.00	K	Joback Method
tc	569.08	K	Joback Method
tf	222.95	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.80	J/molxK	408.00	Joback Method
cpg	171.60	J/molxK	434.85	Joback Method
cpg	178.19	J/molxK	461.69	Joback Method
cpg	184.57	J/molxK	488.54	Joback Method
cpg	190.75	J/molxK	515.38	Joback Method
cpg	196.70	J/molxK	542.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15205660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
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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