

Ethyl methyl sulphone

Other names:	(Methylsulphonyl)ethane Methyl ethyl sulfone
Inchi:	InChI=1S/C3H8O2S/c1-3-6(2,4)5/h3H2,1-2H3
InchiKey:	YBJCDTIWNBNTM-UHFFFAOYSA-N
Formula:	C3H8O2S
SMILES:	CCS(C)(=O)=O
Mol. weight [g/mol]:	108.16
CAS:	594-43-4

Physical Properties

Property code	Value	Unit	Source
chl	-2439.80 ± 0.50	kJ/mol	NIST Webbook
gf	-494.16	kJ/mol	Joback Method
hf	-408.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-486.39 ± 0.71	kJ/mol	NIST Webbook
hfus	14.90	kJ/mol	Joback Method
hvap	78.00 ± 3.00	kJ/mol	NIST Webbook
log10ws	0.09		Crippen Method
logp	0.051		Crippen Method
mcvol	81.220	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
tb	315.82	K	Joback Method
tc	477.89	K	Joback Method
tf	307.70 ± 0.50	K	NIST Webbook
tf	307.70 ± 0.80	K	NIST Webbook
tf	309.00 ± 3.00	K	NIST Webbook
tf	305.70 ± 0.50	K	NIST Webbook
vc	0.330	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.65	J/mol×K	315.82	Joback Method
cpg	133.71	J/mol×K	342.83	Joback Method

cpg	140.60	J/mol×K	369.84	Joback Method
cpg	147.32	J/mol×K	396.86	Joback Method
cpg	153.86	J/mol×K	423.87	Joback Method
cpg	160.23	J/mol×K	450.88	Joback Method
cpg	166.41	J/mol×K	477.89	Joback Method
hfust	11.30	kJ/mol	307.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C594434&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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