1,2-Ethanediol dimethanesulphonate

Other names:	Ethylene glycol, dimethanesulfonate
	Ethylene bis(methanesulfonate)
	Ethylene dimethanesulfonate
	NSC 10716
	1,2-Bis(mesyloxy)ethane
	1,2-Ethanediol dimethanesulfonate
	1,2-Ethanediyl dimethanesulfonate
	Ethane-1,2-diol dimethanesulphonate
	1,2-Ethylene bis(methanesulfonate)
	Dimethylene dimethanesulfonate
	DMSE
	Ethylene methanesulfonate
	EDS
	Methanesulfonic acid, ethylene ester
	NC 429
	Ethane dimethane sulphonate
	1,2-Ethanediol, bismethanesulfonate
	1,2-Ethanediyl methanesulfonate
	Ethylene dimethanesulphonate
	Ethylene-1,2-dimethanesulphonate
	Ethylene glycol dimesylate
Inchi:	InChI=1S/C4H10O6S2/c1-11(5,6)9-3-4-10-12(2,7)8/h3-4H2,1-2H3
InchiKey:	QSQFARNGNIZGAW-UHFFFAOYSA-N
Formula:	C4H10O6S2
SMILES:	CS(=O)(=O)OCCOS(C)(=O)=O
Mol. weight [g/mol]:	218.25
CAS:	4672-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-1164.28	kJ/mol	Joback Method
hf	-1297.03	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	66.59	kJ/mol	Joback Method
log10ws	0.68		Crippen Method
logp	-1.061		Crippen Method

mcvol	135.140	ml/mol	McGowan Method
pc	5687.39	kPa	Joback Method
tb	431.32	K	Joback Method
tc	594.38	K	Joback Method
tf	256.42	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.39	J/mol×K	431.32	Joback Method
cpg	279.84	J/mol×K	458.50	Joback Method
cpg	289.12	J/mol×K	485.67	Joback Method
cpg	298.21	J/mol×K	512.85	Joback Method
cpg	307.09	J/mol×K	540.03	Joback Method
cpg	315.72	J/mol×K	567.20	Joback Method
cpg	324.08	J/mol×K	594.38	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4672495&Units=SI
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

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