Methanesulfonic acid, ethyl ester

Other names:	Ethyl mesylate
	Ethyl methanesulfonate
	EMS
	NSC 26805
	CB 1528
	Ethyl ester of methanesulfonic acid
	Ethyl ester of methylsulfonic acid
	Half-Myleran
	Methylsulfonic acid, ethyl ester
	ENT 26396
	Ethylester kyseliny methansulfonove
	Ethyl ester of methanesulphonic acid
	Ethyl ester of methylsulphonic acid
	Ethyl methanesulphonate
	Ethyl methansulfonate
	Ethyl methansulphonate
	Methanesulphonic acid ethyl ester
	Rcra waste number U119
Inchi:	InChI=1S/C3H8O3S/c1-3-6-7(2,4)5/h3H2,1-2H3
InchiKey:	PLUBXMRUUVWRLT-UHFFFAOYSA-N
Formula:	C3H8O3S
SMILES:	CCOS(C)(=O)=O
Mol. weight [g/mol]:	124.16
CAS:	62-50-0

Physical Properties

Property code	Value	Unit	Source
gf	-599.16	kJ/mol	Joback Method
hf	-690.82	kJ/mol	Joback Method
hfus	16.09	kJ/mol	Joback Method
hvap	43.32	kJ/mol	Joback Method
log10ws	0.01		Crippen Method
logp	-0.017		Crippen Method
mcvol	87.090	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
rinpol	146.35		NIST Webbook
tb	338.24	K	Joback Method

tc	501.95	K	Joback Method
tf	184.36	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.22	J/mol×K	338.24	Joback Method
cpg	154.06	J/mol×K	365.53	Joback Method
cpg	160.80	J/mol×K	392.81	Joback Method
cpg	167.44	J/mol×K	420.10	Joback Method
cpg	173.95	J/mol×K	447.38	Joback Method
cpg	180.33	J/mol×K	474.67	Joback Method
cpg	186.57	J/mol×K	501.95	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62500&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
rinpol: Non-polar retention indices

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