

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	m ³ /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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpola:	Non-polar retention indices

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

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