Methanesulfonic acid, methyl ester

Other names:	Methyl methanesulfonate
	MMS
	as-Dimethyl sulphite
	CB 1540
	FDA 0092
	Methyl ester of methanesulfonic acid
	Methyl mesylate
	Methyl methansulfonate
	Methylmethansulfonat
	NSC-50256
	Methanesulphonic acid methyl ester
	Methylester kyseliny methansulfonove
	Methyl ester of methanesulphonic acid
	Methyl methanesulphonate
	Methyl methansulphonate
Inchi:	InChI=1S/C2H6O3S/c1-5-6(2,3)4/h1-2H3
InchiKey:	MBABOKRGFJTBAE-UHFFFAOYSA-N
Formula:	C2H6O3S
SMILES:	COS(C)(=O)=O
Mol. weight [g/mol]:	110.13
CAS:	66-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-607.58	kJ/mol	Joback Method
hf	-670.18	kJ/mol	Joback Method
hfus	13.50	kJ/mol	Joback Method
hvap	41.09	kJ/mol	Joback Method
log10ws	0.43		Crippen Method
logp	-0.408		Crippen Method
mcvol	73.000	ml/mol	McGowan Method
pc	6180.53	kPa	Joback Method
rinpol	131.02		NIST Webbook
tb	315.36	K	Joback Method
tc	478.40	K	Joback Method
tf	173.09	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.41	J/mol×K	315.36	Joback Method
cpg	122.58	J/mol×K	342.53	Joback Method
cpg	127.72	J/mol×K	369.71	Joback Method
cpg	132.83	J/mol×K	396.88	Joback Method
cpg	137.89	J/mol×K	424.05	Joback Method
cpg	142.88	J/mol×K	451.23	Joback Method
cpg	147.80	J/mol×K	478.40	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66273&Units=SI

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

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