

Methanesulfonic acid, 1-methylethyl ester

Other names:	Methanesulfonic acid, isopropyl ester Isopropyl mesylate Isopropyl methanesulfate Isopropyl methanesulfonate IMS Isopropyl methane sulphonate 2-Propyl methanesulphonate
Inchi:	InChI=1S/C4H10O3S/c1-4(2)7-8(3,5)6/h4H,1-3H3
InchiKey:	SWWHCQCMVCPLEQ-UHFFFAOYSA-N
Formula:	C4H10O3S
SMILES:	CC(C)OS(C)(=O)=O
Mol. weight [g/mol]:	138.19
CAS:	926-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-593.18	kJ/mol	Joback Method
hf	-716.74	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	45.16	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.371		Crippen Method
mcvol	101.180	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	360.68	K	Joback Method
tc	528.48	K	Joback Method
tf	180.63	K	Joback Method
vc	0.398	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.70	J/mol×K	360.68	Joback Method
cpg	188.38	J/mol×K	388.65	Joback Method

cpg	196.88	J/mol×K	416.61	Joback Method
cpg	205.18	J/mol×K	444.58	Joback Method
cpg	213.28	J/mol×K	472.55	Joback Method
cpg	221.17	J/mol×K	500.51	Joback Method
cpg	228.83	J/mol×K	528.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C926067&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

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