

Propanoic acid, 3-methoxy-, methyl ester

Other names:	Methyl «beta»-methoxypropionate Methyl methoxypropionate Methyl 3-methoxypropanoate Methyl 3-methoxypropionate Propionic acid, 3-methoxy-, methyl ester «beta»-Methoxypropionic acid, methyl ester 3-Methoxypropionic acid methyl ester Methylester kyseliny 3-methoxypropionove Methyl ester of 3-methoxypropionic acid Methyl ester of 3-methoxypropanoic acid 3-Methoxypropanoic acid methyl ester NSC 65578
Inchi:	InChI=1S/C5H10O3/c1-7-4-3-5(6)8-2/h3-4H2,1-2H3
InchiKey:	BDJSOPWXYLFTNW-UHFFFAOYSA-N
Formula:	C5H10O3
SMILES:	COCCC(=O)OC
Mol. weight [g/mol]:	118.13
CAS:	3852-09-3

Physical Properties

Property code	Value	Unit	Source
gf	-347.70	kJ/mol	Joback Method
hf	-523.55	kJ/mol	Joback Method
hfus	12.68	kJ/mol	Joback Method
hvap	38.29	kJ/mol	Joback Method
log10ws	0.13		Crippen Method
logp	0.196		Crippen Method
mcvol	94.620	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	412.51	K	Joback Method
tc	591.12	K	Joback Method
tf	240.50	K	Joback Method
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.32	J/mol×K	412.51	Joback Method
cpg	192.64	J/mol×K	442.28	Joback Method
cpg	200.78	J/mol×K	472.05	Joback Method
cpg	208.73	J/mol×K	501.81	Joback Method
cpg	216.48	J/mol×K	531.58	Joback Method
cpg	224.02	J/mol×K	561.35	Joback Method
cpg	231.33	J/mol×K	591.12	Joback Method
dvisc	0.0022410	Pa×s	240.50	Joback Method
dvisc	0.0012761	Pa×s	269.17	Joback Method
dvisc	0.0008098	Pa×s	297.84	Joback Method
dvisc	0.0005566	Pa×s	326.50	Joback Method
dvisc	0.0004065	Pa×s	355.17	Joback Method
dvisc	0.0003111	Pa×s	383.84	Joback Method
dvisc	0.0002471	Pa×s	412.51	Joback Method
hvapt	43.40	kJ/mol	394.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3852093&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
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature

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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