

CH3CHClCH2C(O)OCH3

Other names:	Butanoic acid, 3-chloro-, methyl ester Methyl 3-chlorobutanoate Methyl 3-chlorobutyrate
Inchi:	InChI=1S/C5H9ClO2/c1-4(6)3-5(7)8-2/h4H,3H2,1-2H3
InchiKey:	HDQHWBXUKZBPDN-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	COC(=O)CC(C)Cl
Mol. weight [g/mol]:	136.58
CAS:	817-76-5

Physical Properties

Property code	Value	Unit	Source
chl	-2735.00	kJ/mol	NIST Webbook
gf	-257.07	kJ/mol	Joback Method
hf	-412.35	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	1.177		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	870.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	869.00		NIST Webbook
tb	427.08	K	Joback Method
tc	617.43	K	Joback Method
tf	233.19	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/molxK	427.08	Joback Method
cpg	195.50	J/molxK	458.81	Joback Method
cpg	203.77	J/molxK	490.53	Joback Method
cpg	211.73	J/molxK	522.26	Joback Method
cpg	219.39	J/molxK	553.98	Joback Method
cpg	226.73	J/molxK	585.71	Joback Method
cpg	233.77	J/molxK	617.43	Joback Method
dvisc	0.0042591	Paxs	233.19	Joback Method
dvisc	0.0020958	Paxs	265.50	Joback Method
dvisc	0.0012028	Paxs	297.82	Joback Method
dvisc	0.0007696	Paxs	330.13	Joback Method
dvisc	0.0005332	Paxs	362.45	Joback Method
dvisc	0.0003923	Paxs	394.76	Joback Method
dvisc	0.0003024	Paxs	427.08	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=C817765&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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
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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