

METHYL 3-CHLOROBUTANOATE

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

Physical Properties

Property code	Value	Unit	Source
af	0.3992		Cheméo Relay (1.0)
chl	-2735.00	kJ/mol	NIST Webbook
hf	-490.23	kJ/mol	Cheméo Relay (1.0)
hfus	12.17	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Cheméo Relay (1.0)
ie	10.44	eV	Cheméo Relay (1.0)
log10ws	-1.05		Cheméo Relay (1.0)
logp	1.177		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	881.00		NIST Webbook
rinpol	870.00		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	405.98	K	Cheméo Relay (1.0)
tc	604.13	K	Cheméo Relay (1.0)
tf	223.98	K	Cheméo Relay (1.0)
vc	0.359	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/mol×K	427.08	Joback Method
cpg	233.77	J/mol×K	617.43	Joback Method
cpg	226.73	J/mol×K	585.71	Joback Method
cpg	219.39	J/mol×K	553.98	Joback Method
cpg	211.73	J/mol×K	522.26	Joback Method
cpg	203.77	J/mol×K	490.53	Joback Method
cpg	195.50	J/mol×K	458.81	Joback Method
dvisc	0.0007696	Pa×s	330.13	Joback Method
dvisc	0.0003024	Pa×s	427.08	Joback Method
dvisc	0.0003923	Pa×s	394.76	Joback Method
dvisc	0.0005332	Pa×s	362.45	Joback Method
dvisc	0.0042591	Pa×s	233.19	Joback Method
dvisc	0.0012028	Pa×s	297.82	Joback Method
dvisc	0.0020958	Pa×s	265.50	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C817765&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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