Propanoic acid, 3-chloro-, methyl ester

Other names:	Propionic acid, 3-chloro-, methyl ester
	Methyl 3-chloropropionate
	USAF do-7
Inchi:	InChI=1S/C4H7ClO2/c1-7-4(6)2-3-5/h2-3H2,1H3
InchiKey:	GZGJIACHBCQSPC-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	COC(=O)CCCl
Mol. weight [g/mol]:	122.55
CAS:	6001-87-2

Physical Properties

Property code	Value	Unit	Source
chl	-2098.00	kJ/mol	NIST Webbook
gf	-263.05	kJ/mol	Joback Method
hf	-386.43	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	38.04	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	0.788		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	838.00		NIST Webbook
rinpol	857.30		NIST Webbook
rinpol	825.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	831.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	823.00		NIST Webbook
rinpol	819.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	829.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1339.00		NIST Webbook

ripol	1353.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1339.00		NIST Webbook
tb	429.20	K	NIST Webbook
tc	592.13	K	Joback Method
tf	236.92	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.10	J/mol×K	404.64	Joback Method
cpg	183.10	J/mol×K	560.88	Joback Method
cpg	177.14	J/mol×K	529.63	Joback Method
cpg	170.96	J/mol×K	498.39	Joback Method
cpg	164.55	J/mol×K	467.14	Joback Method
cpg	157.93	J/mol×K	435.89	Joback Method
cpg	188.84	J/mol×K	592.13	Joback Method
dvisc	0.0003259	Pa×s	404.64	Joback Method
dvisc	0.0004081	Pa×s	376.69	Joback Method
dvisc	0.0005298	Pa×s	348.73	Joback Method
dvisc	0.0007199	Pa×s	320.78	Joback Method
dvisc	0.0010371	Pa×s	292.83	Joback Method
dvisc	0.0016136	Pa×s	264.87	Joback Method
dvisc	0.0027868	Pa×s	236.92	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6001872&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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