

3-Chloropentanoic acid, methyl ester

Other names:	Methyl 3-chloropentanoate
Inchi:	InChI=1S/C6H11ClO2/c1-3-5(7)4-6(8)9-2/h5H,3-4H2,1-2H3
InchiKey:	URAPLJYYCURDSC-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CCC(Cl)CC(=O)OC
Mol. weight [g/mol]:	150.60
CAS:	819-92-1

Physical Properties

Property code	Value	Unit	Source
gf	-248.65	kJ/mol	Joback Method
hf	-432.99	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	966.00		NIST Webbook
ripol	1397.00		NIST Webbook
tb	449.96	K	Joback Method
tc	638.50	K	Joback Method
tf	244.46	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.04	J/molxK	449.96	Joback Method
cpg	234.96	J/molxK	481.38	Joback Method
cpg	244.50	J/molxK	512.81	Joback Method
cpg	253.66	J/molxK	544.23	Joback Method
cpg	262.46	J/molxK	575.65	Joback Method
cpg	270.88	J/molxK	607.08	Joback Method

cpg	278.93	J/molxK	638.50	Joback Method
dvisc	0.0043249	Paxs	244.46	Joback Method
dvisc	0.0020836	Paxs	278.71	Joback Method
dvisc	0.0011778	Paxs	312.96	Joback Method
dvisc	0.0007450	Paxs	347.21	Joback Method
dvisc	0.0005117	Paxs	381.46	Joback Method
dvisc	0.0003739	Paxs	415.71	Joback Method
dvisc	0.0002866	Paxs	449.96	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=C819921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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