

3-Chloropropanoic acid, 2-pentyl ester

Other names:	Propanoic acid, 3-chloro, 1-methylbutyl ester
Inchi:	InChI=1S/C8H15ClO2/c1-3-4-7(2)11-8(10)5-6-9/h7H,3-6H2,1-2H3
InchiKey:	ZODXJJOAYWVAGY-UHFFFAOYSA-N
Formula:	C8H15ClO2
SMILES:	CCCC(C)OC(=O)CCCI
Mol. weight [g/mol]:	178.66
CAS:	88736-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-231.81	kJ/mol	Joback Method
hf	-474.27	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.347		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1135.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1114.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1538.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1548.00		NIST Webbook
tb	495.72	K	Joback Method
tc	680.38	K	Joback Method
tf	267.00	K	Joback Method
vc	0.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.89	J/molxK	495.72	Joback Method
cpg	320.07	J/molxK	526.50	Joback Method
cpg	331.75	J/molxK	557.27	Joback Method
cpg	342.95	J/molxK	588.05	Joback Method
cpg	353.67	J/molxK	618.82	Joback Method
cpg	363.91	J/molxK	649.60	Joback Method
cpg	373.67	J/molxK	680.38	Joback Method
dvisc	0.0042242	Paxs	267.00	Joback Method
dvisc	0.0019599	Paxs	305.12	Joback Method
dvisc	0.0010785	Paxs	343.24	Joback Method
dvisc	0.0006687	Paxs	381.36	Joback Method
dvisc	0.0004523	Paxs	419.48	Joback Method
dvisc	0.0003265	Paxs	457.60	Joback Method
dvisc	0.0002478	Paxs	495.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88736678&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
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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