Pentyl 3-chlorobutanoate

Other names: Butanoic acid, 3-chloro, pentyl ester
Inchi: InChI=1S/C9H17ClO2/c1-3-4-5-6-12-9(11)7-8(2)10/h8H,3-7H2,1-2H3
InchiKey: XZQIKQRUJMEJAJ-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 192.68

Physical Properties

Property code	Value	Unit	Source
gf	-223.39	kJ/mol	Joback Method
hf	-494.91	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.737		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1227.00		NIST Webbook
tb	518.60	K	Joback Method
tc	701.32	K	Joback Method
tf	278.27	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.38	J/mol×K	518.60	Joback Method
cpg	365.50	J/mol×K	549.05	Joback Method

cpg	378.08	J/mol×K	579.51	Joback Method
cpg	390.13	J/mol×K	609.96	Joback Method
cpg	401.64	J/mol×K	640.41	Joback Method
cpg	412.64	J/mol×K	670.86	Joback Method
cpg	423.11	J/mol×K	701.32	Joback Method
dvisc	0.0040831	Pa×s	278.27	Joback Method
dvisc	0.0018630	Pa×s	318.32	Joback Method
dvisc	0.0010130	Pa×s	358.38	Joback Method
dvisc	0.0006226	Pa×s	398.44	Joback Method
dvisc	0.0004182	Pa×s	438.49	Joback Method
dvisc	0.0003003	Pa×s	478.55	Joback Method
dvisc	0.0002269	Pa×s	518.60	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28401&Units=SI

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