Propanoic acid, 2-chloro, hexyl ester

Other names: Hexyl 2-chloropropanoate
Inchi: InChI=1S/C9H17ClO2/c1-3-4-5-6-7-12-9(11)8(2)10/h8H,3-7H2,1-2H3
InchiKey: CKKHJCOIGGVMAZ-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCCCOC(=O)C(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	1234.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1216.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1625.00		NIST Webbook
ripol	1623.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1577.00		NIST Webbook

ripol	1594.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1649.00		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

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=R23116&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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