3-Chloropropionic acid, hexyl ester

Other names: Propanoic acid, 3-chloro, hexyl ester
Hexyl 3-chloropropanoate
Inchi: InChI=1S/C9H17ClO2/c1-2-3-4-5-8-12-9(11)6-7-10/h2-8H2,1H3
InchiKey: PYOAHWWMEFRKLM-UHFFFAOYSA-N
Formula: C9H17ClO2
SMILES: CCCCCCOC(=O)CCCl
Mol. weight [g/mol]: 192.68
CAS: 63505-49-7

Physical Properties

Property code	Value	Unit	Source
gf	-220.95	kJ/mol	Joback Method
hf	-489.63	kJ/mol	Joback Method
hfus	26.05	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.739		Crippen Method
mcvol	157.350	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1290.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1288.00		NIST Webbook
ripol	1773.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1794.00		NIST Webbook
ripol	1777.00		NIST Webbook
ripol	1777.00		NIST Webbook

ripol	1732.00		NIST Webbook
ripol	1749.00		NIST Webbook
tb	519.04	K	Joback Method
tc	698.13	K	Joback Method
tf	293.27	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.11	J/mol×K	519.04	Joback Method
cpg	411.03	J/mol×K	668.28	Joback Method
cpg	400.25	J/mol×K	638.43	Joback Method
cpg	388.97	J/mol×K	608.58	Joback Method
cpg	377.20	J/mol×K	578.74	Joback Method
cpg	364.91	J/mol×K	548.89	Joback Method
cpg	421.32	J/mol×K	698.13	Joback Method
dvisc	0.0002406	Pa×s	519.04	Joback Method
dvisc	0.0003106	Pa×s	481.41	Joback Method
dvisc	0.0004189	Pa×s	443.78	Joback Method
dvisc	0.0005970	Pa×s	406.15	Joback Method
dvisc	0.0009148	Pa×s	368.53	Joback Method
dvisc	0.0015445	Pa×s	330.90	Joback Method
dvisc	0.0029830	Pa×s	293.27	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C63505497&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