6-Chlorohexanoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C11H21ClO2/c1-9(2)10(3)14-11(13)7-5-4-6-8-12/h9-10H,4-8H2,1-3H3
InchiKey: DQDKDMPCYNRZJX-UHFFFAOYSA-N
Formula: C11H21ClO2
SMILES: CC(C)C(C)OC(=O)CCCCCCl
Mol. weight [g/mol]: 220.74

Physical Properties

Property code	Value	Unit	Source
gf	-208.99	kJ/mol	Joback Method
hf	-541.47	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	52.84	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.373		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	563.92	K	Joback Method
tc	746.42	K	Joback Method
tf	285.81	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.26	J/mol×K	563.92	Joback Method
cpg	462.29	J/mol×K	594.34	Joback Method
cpg	476.66	J/mol×K	624.75	Joback Method
cpg	490.37	J/mol×K	655.17	Joback Method
cpg	503.45	J/mol×K	685.59	Joback Method
cpg	515.90	J/mol×K	716.00	Joback Method
cpg	527.73	J/mol×K	746.42	Joback Method
dvisc	0.0051422	Pa×s	285.81	Joback Method

dvisc	0.0019735	Pa×s	332.16	Joback Method
dvisc	0.0009576	Pa×s	378.51	Joback Method
dvisc	0.0005441	Pa×s	424.87	Joback Method
dvisc	0.0003455	Pa×s	471.22	Joback Method
dvisc	0.0002380	Pa×s	517.57	Joback Method
dvisc	0.0001743	Pa×s	563.92	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=U354725&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