CHLOROMETHYL 4-CHLOROHEXANOATE

Other names: 4-Chlorohexanoic acid, chloromethyl ester
Inchi: InChI=1S/C7H12Cl2O2/c1-2-6(9)3-4-7(10)11-5-8/h6H,2-5H2,1H3
InchiKey: SKALGZTWKDDAHB-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CCC(Cl)CCC(=O)OCCl
Mol. weight [g/mol]: 199.08

Physical Properties

Property code	Value	Unit	Source
hf	-565.19	kJ/mol	Cheméo Relay (1.0)
hfus	21.54	kJ/mol	Joback Method
hvap	57.30	kJ/mol	Cheméo Relay (1.0)
logp	2.524		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
rinpol	1246.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1264.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1837.00		NIST Webbook
ripol	1863.00		NIST Webbook
tb	494.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.96	J/mol×K	510.27	Joback Method
cpg	301.62	J/mol×K	542.29	Joback Method
cpg	311.82	J/mol×K	574.32	Joback Method
cpg	321.54	J/mol×K	606.34	Joback Method
cpg	330.81	J/mol×K	638.37	Joback Method
cpg	339.62	J/mol×K	670.39	Joback Method
cpg	347.98	J/mol×K	702.42	Joback Method

dvisc	0.0037541	Pa×s	285.65	Joback Method
dvisc	0.0018698	Pa×s	323.09	Joback Method
dvisc	0.0010763	Pa×s	360.52	Joback Method
dvisc	0.0006874	Pa×s	397.96	Joback Method
dvisc	0.0004742	Pa×s	435.40	Joback Method
dvisc	0.0003470	Pa×s	472.83	Joback Method
dvisc	0.0002658	Pa×s	510.27	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418559&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature