CHLOROMETHYL 3-CHLOROHEXANOATE

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

Physical Properties

Property code	Value	Unit	Source
hf	-555.72	kJ/mol	Cheméo Relay (1.0)
hfus	21.54	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Cheméo Relay (1.0)
logp	2.524		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
rinpol	1214.00		NIST Webbook
tb	482.43	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

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
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=C80418548&Units=SI

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
tb:	Normal Boiling Point Temperature