CHLOROMETHYL 6-CHLOROHEXANOATE

Other names: 6-Chlorohexanoic acid, chloromethyl ester
Inchi: InChI=1S/C7H12Cl2O2/c8-5-3-1-2-4-7(10)11-6-9/h1-6H2
InchiKey: NFZSDYANLAMKQW-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: O=C(CCCCCCl)OCCl
Mol. weight [g/mol]: 199.08

Physical Properties

Property code	Value	Unit	Source
hf	-552.80	kJ/mol	Cheméo Relay (1.0)
hfus	25.07	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Cheméo Relay (1.0)
ie	10.22	eV	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	2.525		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1341.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1979.00		NIST Webbook
ripol	2002.00		NIST Webbook
tb	505.88	K	Cheméo Relay (1.0)
tc	703.43	K	Cheméo Relay (1.0)
tf	250.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.67	J/mol×K	510.71	Joback Method
cpg	301.04	J/mol×K	542.07	Joback Method
cpg	310.97	J/mol×K	573.42	Joback Method

cpg	320.46	J/mol×K	604.78	Joback Method
cpg	329.52	J/mol×K	636.14	Joback Method
cpg	338.15	J/mol×K	667.50	Joback Method
cpg	346.35	J/mol×K	698.85	Joback Method
dvisc	0.0028037	Pa×s	300.65	Joback Method
dvisc	0.0015651	Pa×s	335.66	Joback Method
dvisc	0.0009754	Pa×s	370.67	Joback Method
dvisc	0.0006596	Pa×s	405.68	Joback Method
dvisc	0.0004746	Pa×s	440.69	Joback Method
dvisc	0.0003585	Pa×s	475.70	Joback Method
dvisc	0.0002814	Pa×s	510.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418571&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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
ie:	Ionization energy
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