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]: 199.07
CAS: 80418-57-1

Physical Properties

Property code	Value	Unit	Source
gf	-249.72	kJ/mol	Joback Method
hf	-464.09	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	49.10	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.525		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1337.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1979.00		NIST Webbook
ripol	2002.00		NIST Webbook
tb	510.71	K	Joback Method
tc	698.85	K	Joback Method
tf	300.65	K	Joback Method
vc	0.549	m3/kmol	Joback Method

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

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

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