Chloromethyl hexanoate

Other names: Hexanoic acid, chloromethyl ester
Inchi: InChI=1S/C7H13ClO2/c1-2-3-4-5-7(9)10-6-8/h2-6H2,1H3
InchiKey: HNUBMUSOXKDQIN-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCCCCC(=O)OCCl
Mol. weight [g/mol]: 164.63
CAS: 66542-51-6

Physical Properties

Property code	Value	Unit	Source
gf	-237.79	kJ/mol	Joback Method
hf	-448.35	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.306		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1084.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1069.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1477.00		NIST Webbook
tb	473.28	K	Joback Method
tc	655.90	K	Joback Method
tf	270.73	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	265.22	J/mol×K	473.28	Joback Method
cpg	276.01	J/mol×K	503.72	Joback Method
cpg	286.40	J/mol×K	534.15	Joback Method
cpg	296.38	J/mol×K	564.59	Joback Method
cpg	305.96	J/mol×K	595.03	Joback Method
cpg	315.13	J/mol×K	625.46	Joback Method
cpg	323.90	J/mol×K	655.90	Joback Method
dvisc	0.0030645	Pa×s	270.73	Joback Method
dvisc	0.0016518	Pa×s	304.49	Joback Method
dvisc	0.0010072	Pa×s	338.25	Joback Method
dvisc	0.0006719	Pa×s	372.00	Joback Method
dvisc	0.0004794	Pa×s	405.76	Joback Method
dvisc	0.0003603	Pa×s	439.52	Joback Method
dvisc	0.0002820	Pa×s	473.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C66542516&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

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

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