Hexyl chloroformate

Other names:	Carbonochloridic acid, hexyl ester
	Hexyl chloridocarbonate
Inchi:	InChI=1S/C7H13ClO2/c1-2-3-4-5-6-10-7(8)9/h2-6H2,1H3
InchiKey:	KIWBRXCOTCXSSZ-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	CCCCCCOC(=O)Cl
Mol. weight [g/mol]:	164.63
CAS:	6092-54-2

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	-2.75		Crippen Method
logp	2.942		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1055.00		NIST Webbook
rinpol	1055.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.70	K	0.90	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6092542&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume