

6-Chlorohexanoyl chloride

Other names:	Hexanoyl chloride, 6-chloro-
Inchi:	InChI=1S/C6H10Cl2O/c7-5-3-1-2-4-6(8)9/h1-5H2
InchiKey:	WZILXAPNPKMOSA-UHFFFAOYSA-N
Formula:	C6H10Cl2O
SMILES:	O=C(Cl)CCCCCI
Mol. weight [g/mol]:	169.05
CAS:	19347-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-153.14	kJ/mol	Joback Method
hf	-311.23	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	44.47	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.551		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
tb	465.41	K	Joback Method
tc	656.83	K	Joback Method
tf	267.15	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.57	J/mol×K	465.41	Joback Method
cpg	236.97	J/mol×K	497.31	Joback Method
cpg	245.93	J/mol×K	529.22	Joback Method
cpg	254.45	J/mol×K	561.12	Joback Method
cpg	262.55	J/mol×K	593.03	Joback Method
cpg	270.23	J/mol×K	624.93	Joback Method
cpg	277.52	J/mol×K	656.83	Joback Method
dvisc	0.0038339	Pa×s	267.15	Joback Method

dvisc	0.0020971	Pa×s	300.19	Joback Method
dvisc	0.0012929	Pa×s	333.24	Joback Method
dvisc	0.0008698	Pa×s	366.28	Joback Method
dvisc	0.0006248	Pa×s	399.32	Joback Method
dvisc	0.0004721	Pa×s	432.37	Joback Method
dvisc	0.0003712	Pa×s	465.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19347730&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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