

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)CCCCCCl
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	m ³ /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	Paxs	267.15	Joback Method

dvisc	0.0020971	Paxs	300.19	Joback Method
dvisc	0.0012929	Paxs	333.24	Joback Method
dvisc	0.0008698	Paxs	366.28	Joback Method
dvisc	0.0006248	Paxs	399.32	Joback Method
dvisc	0.0004721	Paxs	432.37	Joback Method
dvisc	0.0003712	Paxs	465.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19347730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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