Cyclohexanecarbonyl chloride

Other names:	Chlorocarbonylcyclohexane
	Cyclohexanoyl chloride
	Cyclohexylcarbonyl chloride
	Hexahydrobenzoyl chloride
	Cyclohexanecarboxylic acid chloride
Inchi:	InChI=1S/C7H11ClO/c8-7(9)6-4-2-1-3-5-6/h6H,1-5H2
InchiKey:	RVOJTCZRIKWHDX-UHFFFAOYSA-N
Formula:	C7H11ClO
SMILES:	O=C(Cl)C1CCCCC1
Mol. weight [g/mol]:	146.62
CAS:	2719-27-9

Physical Properties

Property code	Value	Unit	Source
gf	-108.34	kJ/mol	Joback Method
hf	-261.81	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	42.74	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.332		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	457.00 ± 3.00	K	NIST Webbook
tb	454.00 ± 4.00	K	NIST Webbook
tb	457.20	K	NIST Webbook
tc	693.24	K	Joback Method
tf	255.88	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.45	J/mol×K	470.41	Joback Method
cpg	239.24	J/mol×K	507.55	Joback Method

cpg	253.16	J/mol×K	544.69	Joback Method
cpg	266.24	J/mol×K	581.82	Joback Method
cpg	278.49	J/mol×K	618.96	Joback Method
cpg	289.96	J/mol×K	656.10	Joback Method
cpg	300.65	J/mol×K	693.24	Joback Method
dvisc	0.0054577	Pa×s	255.88	Joback Method
dvisc	0.0026455	Pa×s	291.63	Joback Method
dvisc	0.0015022	Pa×s	327.39	Joback Method
dvisc	0.0009535	Pa×s	363.14	Joback Method
dvisc	0.0006566	Pa×s	398.90	Joback Method
dvisc	0.0004808	Pa×s	434.65	Joback Method
dvisc	0.0003691	Pa×s	470.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.50 ± 0.50	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2719279&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume