o-Chlorobenzoyl chloride

Other names:	2-Chlorobenzoyl chloride
	Benzoyl chloride, o-chloro-
Inchi:	InChI=1S/C7H4Cl2O/c8-6-4-2-1-3-5(6)7(9)10/h1-4H
InchiKey:	ONIKNECPXCLUHT-UHFFFAOYSA-N
Formula:	C7H4Cl2O
SMILES:	O=C(Cl)c1ccccc1Cl
Mol. weight [g/mol]:	175.01
CAS:	609-65-4

Physical Properties

Property code	Value	Unit	Source
af	0.4294		Cheméo Relay (1.0)
gf	-41.94	kJ/mol	Joback Method
hf	-137.26	kJ/mol	Cheméo Relay (1.0)
hfl	-171.50 ± 0.79	kJ/mol	NIST Webbook
hfus	17.53	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-2.84		Cheméo Relay (1.0)
logp	2.719		Crippen Method
mcvol	111.780	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	511.20	K	NIST Webbook
tc	749.72	K	Cheméo Relay (1.0)
tf	263.49	K	Cheméo Relay (1.0)
vc	0.403	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.90	J/mol×K	718.56	Joback Method
cpg	239.57	J/mol×K	758.29	Joback Method
cpg	205.65	J/mol×K	559.67	Joback Method
cpg	213.61	J/mol×K	599.40	Joback Method

cpg	220.95	J/mol×K	639.12	Joback Method
cpg	227.70	J/mol×K	678.84	Joback Method
cpg	197.03	J/mol×K	519.95	Joback Method
dvisc	0.0009150	Pa×s	384.89	Joback Method
dvisc	0.0013446	Pa×s	351.12	Joback Method
dvisc	0.0021445	Pa×s	317.36	Joback Method
dvisc	0.0006626	Pa×s	418.66	Joback Method
dvisc	0.0005035	Pa×s	452.42	Joback Method
dvisc	0.0003974	Pa×s	486.19	Joback Method
dvisc	0.0003235	Pa×s	519.95	Joback Method
hvapt	53.40	kJ/mol	384.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.20133e+01
Coeff. B	-2.99903e+03
Coeff. C	-1.16234e+02
Temperature range (K), min.	366.15
Temperature range (K), max.	563.73

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C609654&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume