Benzoyl chloride, 4-chloro-

Other names:	4-Chlorobenzoic acid chloride
	4-Chlorobenzoyl chloride
	Benzoyl chloride, p-chloro-
	p-Chlorobenzoyl chloride
	para-Chlorobenzoyl chloride
Inchi:	InChI=1S/C7H4Cl2O/c8-6-3-1-5(2-4-6)7(9)10/h1-4H
InchiKey:	RKIDDEGICSMIJA-UHFFFAOYSA-N
Formula:	C7H4Cl2O
SMILES:	O=C(Cl)c1ccc(Cl)cc1
Mol. weight [g/mol]:	175.01
CAS:	122-01-0

Physical Properties

Property code	Value	Unit	Source
gf	-41.94	kJ/mol	Joback Method
hf	-128.90 ± 4.30	kJ/mol	NIST Webbook
hfl	-190.90 ± 0.88	kJ/mol	NIST Webbook
hfl	-191.70 ± 1.10	kJ/mol	NIST Webbook
hfus	17.53	kJ/mol	Joback Method
hvap	49.63	kJ/mol	Joback Method
ie	9.58 ± 0.03	eV	NIST Webbook
log10ws	-3.05		Crippen Method
logp	2.719		Crippen Method
mcvol	111.780	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	495.20	K	NIST Webbook
tc	758.29	K	Joback Method
tf	317.36	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.57	J/mol×K	758.29	Joback Method

cpg	233.90	J/mol×K	718.56	Joback Method
cpg	227.70	J/mol×K	678.84	Joback Method
cpg	220.95	J/mol×K	639.12	Joback Method
cpg	213.61	J/mol×K	599.40	Joback Method
cpg	205.65	J/mol×K	559.67	Joback Method
cpg	197.03	J/mol×K	519.95	Joback Method
dvisc	0.0021445	Pa×s	317.36	Joback Method
dvisc	0.0003235	Pa×s	519.95	Joback Method
dvisc	0.0003974	Pa×s	486.19	Joback Method
dvisc	0.0005035	Pa×s	452.42	Joback Method
dvisc	0.0006626	Pa×s	418.66	Joback Method
dvisc	0.0009150	Pa×s	384.89	Joback Method
dvisc	0.0013446	Pa×s	351.12	Joback Method
hvapt	55.70	kJ/mol	381.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56902e+01
Coeff. B	-5.77711e+03
Temperature range (K), min.	370.00
Temperature range (K), max.	556.63

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122010&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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