Benzoyl chloride

Other names:	ALPHA-CHLORO-BENZALDEHYDE
	BENZENECARBONYL CHLORIDE
	Benzaldehyde, «alpha»-chloro-
	Benzaldehyde, Â«alphaÂ»-chloro-
	Benzoic acid, chloride
	UN 1736
	«alpha»-Chlorobenzaldehyde
	Â«alphaÂ»-Chlorobenzaldehyde
Inchi:	InChI=1S/C7H5ClO/c8-7(9)6-4-2-1-3-5-6/h1-5H
InchiKey:	PASDCCFISLVPSO-UHFFFAOYSA-N
Formula:	C7H5ClO
SMILES:	O=C(Cl)c1ccccc1
Mol. weight [g/mol]:	140.57
CAS:	98-88-4

Physical Properties

Property code	Value	Unit	Source
chl	-3332.60	kJ/mol	NIST Webbook
gf	-20.38	kJ/mol	Joback Method
hf	-109.00 ± 4.20	kJ/mol	NIST Webbook
hfl	-160.30	kJ/mol	NIST Webbook
hfl	-157.30 ± 0.40	kJ/mol	NIST Webbook
hfl	-164.40	kJ/mol	NIST Webbook
hfus	13.72	kJ/mol	Joback Method
hvap	54.80 ± 4.20	kJ/mol	NIST Webbook
ie	9.70 ± 0.01	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.92	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
ie	9.54	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.69	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	2.066		Crippen Method

mcvol	99.540	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	1080.00		NIST Webbook
rinpol	1036.50		NIST Webbook
rinpol	1095.10		NIST Webbook
rinpol	1046.00		NIST Webbook
rinpol	1038.00		NIST Webbook
tb	470.40	K	NIST Webbook
tb	470.35 ± 0.50	K	NIST Webbook
tb	472.20 ± 3.00	K	NIST Webbook
tb	471.00 ± 3.00	K	NIST Webbook
tb	469.85	K	KDB
tb	469.00 ± 3.00	K	NIST Webbook
tb	471.00 ± 7.00	K	NIST Webbook
tb	471.00	K	NIST Webbook
tb	470.00	K	NIST Webbook
tc	709.16	K	Joback Method
tf	272.75 ± 0.20	K	NIST Webbook
tf	272.55	K	KDB
tf	272.00	K	NIST Webbook
tf	272.52 ± 0.35	K	NIST Webbook
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.31	J/mol×K	670.55	Joback Method
cpg	176.16	J/mol×K	477.54	Joback Method
cpg	185.94	J/mol×K	516.14	Joback Method
cpg	195.02	J/mol×K	554.75	Joback Method
cpg	203.42	J/mol×K	593.35	Joback Method
cpg	211.17	J/mol×K	631.95	Joback Method
cpg	224.88	J/mol×K	709.16	Joback Method
cpl	187.00	J/mol×K	298.00	NIST Webbook
dvisc	0.0003211	Pa×s	477.54	Joback Method
dvisc	0.0028759	Pa×s	274.92	Joback Method
dvisc	0.0016342	Pa×s	308.69	Joback Method
dvisc	0.0010381	Pa×s	342.46	Joback Method
dvisc	0.0007154	Pa×s	376.23	Joback Method
dvisc	0.0005242	Pa×s	410.00	Joback Method
dvisc	0.0004027	Pa×s	443.77	Joback Method

hvapt	49.60	kJ/mol	387.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61165e+01
Coeff. B	-4.88082e+03
Coeff. C	-3.73660e+01
Temperature range (K), min.	345.72
Temperature range (K), max.	489.08

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1692.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98884&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume