2,6-Dichlorobenzoyl chloride

Other names: Benzoyl chloride, 2,6-dichloro-
Inchi: InChI=1S/C7H3Cl3O/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H
InchiKey: JBLIDPPHFGWTKU-UHFFFAOYSA-N
Formula: C7H3Cl3O
SMILES: O=C(Cl)c1c(Cl)cccc1Cl
Mol. weight [g/mol]: 209.46
CAS: 4659-45-4

Physical Properties

Property code	Value	Unit	Source
gf	-63.50	kJ/mol	Joback Method
hf	-134.02	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.372		Crippen Method
mcvol	124.020	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
tb	562.36	K	Joback Method
tc	806.32	K	Joback Method
tf	359.80	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.68	J/mol×K	562.36	Joback Method
cpg	223.19	J/mol×K	603.02	Joback Method
cpg	230.11	J/mol×K	643.68	Joback Method
cpg	236.47	J/mol×K	684.34	Joback Method
cpg	242.29	J/mol×K	725.00	Joback Method
cpg	247.61	J/mol×K	765.66	Joback Method
cpg	252.44	J/mol×K	806.32	Joback Method
dvisc	0.0016548	Pa×s	359.80	Joback Method

dvisc	0.0011138	Pa×s	393.56	Joback Method
dvisc	0.0007980	Pa×s	427.32	Joback Method
dvisc	0.0006004	Pa×s	461.08	Joback Method
dvisc	0.0004696	Pa×s	494.84	Joback Method
dvisc	0.0003790	Pa×s	528.60	Joback Method
dvisc	0.0003139	Pa×s	562.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.70	K	2.80	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4659454&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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