Benzoyl chloride, 3,4-dichloro-

Other names:	3,4-Dichlorobenzoyl chloride
Inchi:	InChI=1S/C7H3Cl3O/c8-5-2-1-4(7(10)11)3-6(5)9/h1-3H
InchiKey:	VTXNOVCTHUBABW-UHFFFAOYSA-N
Formula:	C7H3Cl3O
SMILES:	O=C(Cl)c1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]:	209.46
CAS:	3024-72-4

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	515.20	K	NIST Webbook
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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3024724&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/52-685-4/Benzoyl-chloride-3-4-dichloro.pdf
Generated by Cheméo on 2024-10-12 08:19:47.068428632 +0000 UTC m=+3302049.705397879.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.