

Benzoyl chloride, 2,4-dichloro-

Other names:	2,4-Dichlorobenzoyl chloride
Inchi:	InChI=1S/C7H3Cl3O/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H
InchiKey:	CEOCVKWBUWKBKA-UHFFFAOYSA-N
Formula:	C7H3Cl3O
SMILES:	O=C(Cl)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	209.46
CAS:	89-75-8

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.68	J/mol×K	562.36	Joback Method
cpg	247.61	J/mol×K	765.66	Joback Method
cpg	242.29	J/mol×K	725.00	Joback Method
cpg	236.47	J/mol×K	684.34	Joback Method
cpg	230.11	J/mol×K	643.68	Joback Method
cpg	223.19	J/mol×K	603.02	Joback Method
cpg	252.44	J/mol×K	806.32	Joback Method
dvisc	0.0003139	Paxs	562.36	Joback Method

dvisc	0.0003790	Paxs	528.60	Joback Method
dvisc	0.0004696	Paxs	494.84	Joback Method
dvisc	0.0006004	Paxs	461.08	Joback Method
dvisc	0.0007980	Paxs	427.32	Joback Method
dvisc	0.0011138	Paxs	393.56	Joback Method
dvisc	0.0016548	Paxs	359.80	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	4.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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