

Benzoic acid, 2,6-dichloro-

Other names:	2,6-Dichlorobenzoic acid
Inchi:	InChI=1S/C7H4Cl2O2/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3H,(H,10,11)
InchiKey:	MRUDNSFOFOQZDA-UHFFFAOYSA-N
Formula:	C7H4Cl2O2
SMILES:	O=C(O)c1c(Cl)cccc1Cl
Mol. weight [g/mol]:	191.01
CAS:	50-30-6

Physical Properties

Property code	Value	Unit	Source
gf	-188.39	kJ/mol	Joback Method
hf	-270.51	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	66.97	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.692		Crippen Method
mcvol	117.650	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	617.11	K	Joback Method
tc	836.94	K	Joback Method
tf	415.00 ± 2.00	K	NIST Webbook
vc	0.443	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.22	J/mol×K	617.11	Joback Method
cpg	259.93	J/mol×K	800.30	Joback Method
cpg	255.05	J/mol×K	763.66	Joback Method
cpg	249.76	J/mol×K	727.03	Joback Method
cpg	244.04	J/mol×K	690.39	Joback Method
cpg	237.87	J/mol×K	653.75	Joback Method
cpg	264.41	J/mol×K	836.94	Joback Method
dvisc	0.0001057	Paxs	617.11	Joback Method

dvisc	0.0001483	Paxs	579.38	Joback Method
dvisc	0.0002182	Paxs	541.64	Joback Method
dvisc	0.0003400	Paxs	503.90	Joback Method
dvisc	0.0005693	Paxs	466.17	Joback Method
dvisc	0.0010438	Paxs	428.44	Joback Method
dvisc	0.0021517	Paxs	390.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50306&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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