2,4-DICHLOROBENZOIC ACID

Other names: benzoic acid, 2,4-dichloro-
Inchi: InChI=1S/C7H4Cl2O2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,(H,10,11)
InchiKey: ATCRIUVQKHMXSH-UHFFFAOYSA-N
Formula: C7H4Cl2O2
SMILES: O=C(O)c1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 191.01

Physical Properties

Property code	Value	Unit	Source
hf	-347.54	kJ/mol	Cheméo Relay (1.0)
hfus	21.23	kJ/mol	Joback Method
hvap	91.04	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-2.93		Cheméo Relay (1.0)
logp	2.692		Crippen Method
mcvol	117.650	ml/mol	McGowan Method
tb	551.13	K	Cheméo Relay (1.0)
tf	409.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.22	J/mol×K	617.11	Joback Method
cpg	237.87	J/mol×K	653.75	Joback Method
cpg	244.04	J/mol×K	690.39	Joback Method
cpg	249.76	J/mol×K	727.03	Joback Method
cpg	255.05	J/mol×K	763.66	Joback Method
cpg	259.93	J/mol×K	800.30	Joback Method
cpg	264.41	J/mol×K	836.94	Joback Method
dvisc	0.0021517	Pa×s	390.70	Joback Method
dvisc	0.0010438	Pa×s	428.44	Joback Method
dvisc	0.0005693	Pa×s	466.17	Joback Method
dvisc	0.0003400	Pa×s	503.91	Joback Method
dvisc	0.0002182	Pa×s	541.64	Joback Method

dvisc	0.0001483	Pa×s	579.38	Joback Method
dvisc	0.0001057	Pa×s	617.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility of 3,5-Dimethoxybenzoic Acid, 4-Cyanobenzoic Acid, 4-Acetoxybenzoic Acid, 3,5-Diaminobenzoic Acid, and 2,4-Dichlorobenzoic Acid in Ethanol:	https://www.doi.org/10.1021/je900190n
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50840&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point