

Benzoic acid, 2,5-dichloro-

Other names:	2,5-Dichlorobenzoic acid
Inchi:	InChI=1S/C7H4Cl2O2/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3H,(H,10,11)
InchiKey:	QVTQYSFCFOGITD-UHFFFAOYSA-N
Formula:	C7H4Cl2O2
SMILES:	O=C(O)c1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	191.01
CAS:	50-79-3

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	574.20	K	NIST Webbook
tc	836.94	K	Joback Method
tf	427.65 ± 1.00	K	NIST Webbook
tf	426.65 ± 1.00	K	NIST Webbook
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0021517	Paxs	390.70	Joback Method
dvisc	0.0010438	Paxs	428.44	Joback Method
dvisc	0.0005693	Paxs	466.17	Joback Method
dvisc	0.0003400	Paxs	503.90	Joback Method
dvisc	0.0002182	Paxs	541.64	Joback Method
dvisc	0.0001483	Paxs	579.38	Joback Method
dvisc	0.0001057	Paxs	617.11	Joback Method

Sources

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=C50793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/50-453-3/Benzoic-acid-2-5-dichloro.pdf>

Generated by Cheméo on 2024-04-24 22:19:26.931649008 +0000 UTC m=+16286415.852226320.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.