

3,6-Dichloropicolinic acid

Inchi:	InChI=1S/C6H3Cl2NO2/c7-3-1-2-4(8)9-5(3)6(10)11/h1-2H,(H,10,11)
InchiKey:	HUBANNPOLNYSAD-UHFFFAOYSA-N
Formula:	C6H3Cl2NO2
SMILES:	O=C(O)c1nc(Cl)ccc1Cl
Mol. weight [g/mol]:	192.00
CAS:	1702-17-6

Physical Properties

Property code	Value	Unit	Source
logp	2.087		Crippen Method
mcvol	113.540	ml/mol	McGowan Method
tb	555.99	K	Cheméo Relay (1.0)
tf	424.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

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):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/110-305-0/3-6-Dichloropicolinic-acid.pdf>

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