

2,6-Dichloro-4-trifluoromethylpyridine

Inchi:	InChI=1S/C6H2Cl2F3N/c7-4-1-3(6(9,10)11)2-5(8)12-4/h1-2H
InchiKey:	KVNQWVYYVLCZKK-UHFFFAOYSA-N
Formula:	C6H2Cl2F3N
SMILES:	FC(F)(F)c1cc(Cl)nc(Cl)c1
Mol. weight [g/mol]:	215.99
CAS:	39890-98-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	3.407		Crippen Method
mcvol	111.410	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39890987&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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