

4-Hydroxy-2-trifluoromethylpyrimidine

Inchi:	InChI=1S/C5H3F3N2O/c6-5(7,8)4-9-2-1-3(11)10-4/h1-2H,(H,9,10,11)
InchiKey:	PDCVDVCPQWFGAX-UHFFFAOYSA-N
Formula:	C5H3F3N2O
SMILES:	Oc1ccnc(C(F)(F)F)n1
Mol. weight [g/mol]:	164.09
CAS:	1546-80-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Crippen Method
logp	1.201		Crippen Method
mcvol	88.690	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=C1546801&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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<https://www.chemeo.com/cid/11-456-3/4-Hydroxy-2-trifluoromethylpyrimidine.pdf>

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