

2-Amino-4-hydroxy-6-(trifluoromethyl)pyrimidine

Inchi:	InChI=1S/C5H4F3N3O/c6-5(7,8)2-1-3(12)11-4(9)10-2/h1H,(H3,9,10,11,12)
InchiKey:	ZEPSVMLZBXDPGU-UHFFFAOYSA-N
Formula:	C5H4F3N3O
SMILES:	<chem>N=c1nc(O)cc(C(F)(F)F)[nH]1</chem>
Mol. weight [g/mol]:	179.10
CAS:	1513-69-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.10		Crippen Method
logp	0.132		Crippen Method
mcvol	98.670	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1513695&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/96-760-2/2-Amino-4-hydroxy-6-trifluoromethyl-pyrimidine.pdf>

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