

Uracil, 6-(trifluoromethyl)-

Other names:	Uracil, 6-(trifluoromethyl)- 6-(Trifluoromethyl)uracil
Inchi:	InChI=1S/C5H3F3N2O2/c6-5(7,8)2-1-3(11)10-4(12)9-2/h1H,(H2,9,10,11,12)
InchiKey:	IROWWTVZNHKLLE-UHFFFAOYSA-N
Formula:	C5H3F3N2O2
SMILES:	Oc1cc(C(F)(F)F)nc(O)n1
Mol. weight [g/mol]:	180.08

Physical Properties

Property code	Value	Unit	Source
logp	0.907		Crippen Method
mcvol	94.560	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C672457&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/29-858-8/Uracil-6-trifluoromethyl.pdf>

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