

# 2,4(1H,3H)-Pyrimidinedione, 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:	IROWWTVZNHKLLU-UHFFFAOYSA-N
Formula:	C5H3F3N2O2
SMILES:	Oc1cc(C(F)(F)F)nc(O)n1
Mol. weight [g/mol]:	180.08
CAS:	672-45-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.20		Crippen Method
logp	0.907		Crippen Method
mcvol	94.560	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C672457&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C672457&amp;Units=SI</a>

## Legend

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

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