

Pyrimidine, 2,4,6-trifluoro-

Other names:	2,4,6-Trifluoropyrimidine
Inchi:	InChI=1S/C4HF3N2/c5-2-1-3(6)9-4(7)8-2/h1H
InchiKey:	NTSYSQNAPGMSIH-UHFFFAOYSA-N
Formula:	C4HF3N2
SMILES:	Fc1cc(F)nc(F)n1
Mol. weight [g/mol]:	134.06
CAS:	696-82-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.00		Crippen Method
logp	0.894		Crippen Method
mcvol	68.730	ml/mol	McGowan Method

Sources

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=C696822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/72-913-8/Pyrimidine-2-4-6-trifluoro.pdf>

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