

Pyrimidine,4,6-difluoro-

Other names:	4,6-Difluoro-pyrimidine
Inchi:	InChI=1S/C4H2F2N2/c5-3-1-4(6)8-2-7-3/h1-2H
InchiKey:	MCLDVUCSDZGNRR-UHFFFAOYSA-N
Formula:	C4H2F2N2
SMILES:	Fc1cc(F)ncn1
Mol. weight [g/mol]:	116.07
CAS:	2802-62-2

Physical Properties

Property code	Value	Unit	Source
ie	10.95	eV	NIST Webbook
log10ws	-1.67		Crippen Method
logp	0.755		Crippen Method
mcvol	66.960	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2802622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

ie:	Ionization energy
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/120-863-0/Pyrimidine-4-6-difluoro.pdf>

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