

Pyrimidine,2,4-difluoro-

Other names:	2,4-Difluoro-pyrimidine
Inchi:	InChI=1S/C4H2F2N2/c5-3-1-2-7-4(6)8-3/h1-2H
InchiKey:	JZSYSXZDIQUOGP-UHFFFAOYSA-N
Formula:	C4H2F2N2
SMILES:	Fc1ccnc(F)n1
Mol. weight [g/mol]:	116.07
CAS:	2802-61-1

Physical Properties

Property code	Value	Unit	Source
ie	10.65	eV	NIST Webbook
log10ws	-1.67		Crippen Method
logp	0.755		Crippen Method
mcvol	66.960	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2802611&Units=SI

Legend

ie:	Ionization energy
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/14-361-5/Pyrimidine-2-4-difluoro.pdf>

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