

Benzimidazole, 4-acetamido-5,7-difluoro-

Inchi:	InChI=1S/C9H7F2N3O/c1-4(15)14-8-6(11)2-5(10)7-9(8)13-3-12-7/h2-3H,1H3,(H,12,13)(H,14)
InchiKey:	RSGYOISXIYGAOV-UHFFFAOYSA-N
Formula:	C9H7F2N3O
SMILES:	CC(=O)Nc1c(F)cc(F)c2nc[nH]c12
Mol. weight [g/mol]:	211.17
CAS:	4140-71-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.13		Crippen Method
logp	1.318		Crippen Method
mcvol	133.800	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=C4140710&Units=SI

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/55-440-2/Benzimidazole-4-acetamido-5-7-difluoro.pdf>

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