

Acetamide, n-(5,7-difluoro-1h-benzotriazol-4-yl)-

Inchi: InChI=1S/C8H6F2N4O/c1-3(15)11-6-4(9)2-5(10)7-8(6)13-14-12-7/h2H,1H3,(H,11,15)(H,
InchiKey: VVWABZRYJMUANY-UHFFFAOYSA-N
Formula: C8H6F2N4O
SMILES: CC(=O)Nc1c(F)cc(F)c2[nH]nnc12
Mol. weight [g/mol]: 212.16
CAS: 4140-72-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.89		Crippen Method
logp	0.713		Crippen Method
mcvol	129.690	ml/mol	McGowan Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4140721&Units=SI>

Legend

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

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