

N-(2-Furoyl)aminopurine

Inchi:	InChI=1S/C10H7N5O2/c16-10(8-2-1-3-17-8)14-15-4-7-9(13-6-15)12-5-11-7/h1-6H,(H,14)
InchiKey:	OFENXJXBEDNADN-UHFFFAOYSA-N
Formula:	C10H7N5O2
SMILES:	O=C(Nn1cnc2ncnc-2c1)c1ccco1
Mol. weight [g/mol]:	229.19
CAS:	65316-39-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.95		Crippen Method
logp	0.755		Crippen Method
mcvol	150.720	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=C65316394&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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