

Purin-2-ol, 6-dimethylamino-

Inchi:	InChI=1S/C7H9N5O/c1-12(2)6-4-5(9-3-8-4)10-7(13)11-6/h3H,1-2H3,(H2,8,9,10,11,13)
InchiKey:	OTMUNAGWUBKJPP-UHFFFAOYSA-N
Formula:	C7H9N5O
SMILES:	CN(C)c1nc(O)nc2nc[nH]c12
Mol. weight [g/mol]:	179.18
CAS:	24391-36-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	-0.357		Crippen Method
mcvol	126.340	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24391364&Units=SI
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

Legend

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

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