

1-Pentanol, 2,2-dimethyl-5-(6-purinylamino)-

Inchi:	InChI=1S/C12H19N5O/c1-12(2,6-18)4-3-5-13-10-9-11(15-7-14-9)17-8-16-10/h7-8,18H,3
InchiKey:	WGGUVIVLEMPPER-UHFFFAOYSA-N
Formula:	C12H19N5O
SMILES:	CC(C)(CO)CCCNc1nc[nH]c2ncnc1-2
Mol. weight [g/mol]:	249.31
CAS:	19270-93-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Crippen Method
logp	1.033		Crippen Method
mcvol	196.790	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19270930&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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