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/ci990307l
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