

6-Benzylaminopurine, N-pentafluoropropionyl-

Inchi: InChI=1S/C15H10F5N5O/c16-14(17,15(18,19)20)13(26)25(6-9-4-2-1-3-5-9)12-10-11(22-
InchiKey: MUCYPININDNSRP-UHFFFAOYSA-N
Formula: C15H10F5N5O
SMILES: O=C(N(Cc1ccccc1)c1ncnc2nc[nH]c12)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 371.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	2.602		Crippen Method
mcvol	219.850	ml/mol	McGowan Method
rinpol	2460.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U374453&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
rinpol: Non-polar retention indices

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