6-Benzylaminopurine, N-heptafluorobutyryl-

Inchi: InChI=1S/C16H10F7N5O/c17-14(18,15(19,20)16(21,22)23)13(29)28(6-9-4-2-1-3-5-9)12-
InchiKey: FZAPIODDYRMZKS-UHFFFAOYSA-N
Formula: C16H10F7N5O
SMILES: O=C(N(Cc1ccccc1)c1ncnc2nc[nH]c12)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 421.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.13		Crippen Method
logp	3.237		Crippen Method
mcvol	237.480	ml/mol	McGowan Method
rinpol	2469.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374771&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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