Norharmane, N-pentafluoropropionyl-

Inchi: InChI=1S/C14H7F5N2O/c15-13(16,14(17,18)19)12(22)21-10-4-2-1-3-8(10)9-5-6-20-7-11
InchiKey: JQMLUBIYBCATFT-UHFFFAOYSA-N
Formula: C14H7F5N2O
SMILES: O=C(n1c2ccccc2c2ccncc21)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 314.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.36		Crippen Method
logp	4.027		Crippen Method
mcvol	180.120	ml/mol	McGowan Method
rinpol	1827.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374756&Units=SI

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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