

Norharmane, N-heptafluorobutyryl-

Inchi: InChI=1S/C15H7F7N2O/c16-13(17,14(18,19)15(20,21)22)12(25)24-10-4-2-1-3-8(10)9-5-
InchiKey: DTQQDOIDSFLWKC-UHFFFAOYSA-N
Formula: C15H7F7N2O
SMILES: O=C(n1c2ccccc2c2ccncc21)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 364.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	4.663		Crippen Method
mcvol	197.750	ml/mol	McGowan Method
rinpole	1854.00		NIST Webbook

Sources

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=U374460&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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