Norharmane, N-trifluoroacetyl-

Inchi: InChI=1S/C13H7F3N2O/c14-13(15,16)12(19)18-10-4-2-1-3-8(10)9-5-6-17-7-11(9)18/h1-
InchiKey: IDOLYMJWNVEONA-UHFFFAOYSA-N
Formula: C13H7F3N2O
SMILES: O=C(n1c2ccccc2c2ccncc21)C(F)(F)F
Mol. weight [g/mol]: 264.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	3.392		Crippen Method
mcvol	162.490	ml/mol	McGowan Method
rinpol	1848.00		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=U374787&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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