

1-(8-Bromo-dibenzo[1,2-b; 4,5-b']difuran-4-yl-2-aminopropane, N-methyl, TFA

InChIKey:

InChI=1S/C16H13BrF3NO3/c1-8(21(2)15(22)16(18,19)20)7-11-9-3-5-24-14(9)12(17)10-4

Formula:

C16H13BrF3NO3

SMILES:

CC(Cc1c2ccoc2c(Br)c2ccoc12)N(C)C(=O)C(F)(F)F

Mol. weight [g/mol]:

404.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-15.31		Crippen Method
logp	4.893		Crippen Method
mcvol	228.320	ml/mol	McGowan Method
rinpol	2230.00		NIST Webbook
rinpol	2274.00		NIST Webbook
rinpol	2230.00		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=R640565&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
rinpol:	Non-polar retention indices

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