

Triflubazam

Inchi: InChI=1S/C17H13F3N2O2/c1-21-13-8-7-11(17(18,19)20)9-14(13)22(16(24)10-15(21)23)
InchiKey: DMNPCIKBNDKNTU-UHFFFAOYSA-N
Formula: C17H13F3N2O2
SMILES: CN1C(=O)CC(=O)N(c2ccccc2)c2cc(C(F)(F)F)ccc21
Mol. weight [g/mol]: 334.29
CAS: 22365-40-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	3.737		Crippen Method
mcvol	220.420	ml/mol	McGowan Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C22365408&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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<https://www.chemeo.com/cid/37-180-1/Triflubazam.pdf>

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