

3,5-Bis(trifluoromethyl)benzeneboronate, mephenesin

Inchi: InChI=1S/C18H15BF6O3/c1-11-4-2-3-5-16(11)26-9-15-10-27-19(28-15)14-7-12(17(20,21)18)3
InchiKey: DOJBYDPEVKKFJC-UHFFFAOYSA-N
Formula: C18H15BF6O3
SMILES: Cc1ccccc1OCC1COB(c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O1
Mol. weight [g/mol]: 404.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.55		Crippen Method
logp	4.222		Crippen Method
rinpol	1972.00		NIST Webbook
rinpol	1972.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R146726&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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