

3,5-Bis(trifluoromethyl)benzeneboronate, guaifenesin

Inchi:	InChI=1S/C18H15BF6O4/c1-26-15-4-2-3-5-16(15)27-9-14-10-28-19(29-14)13-7-11(17(20
InchiKey:	ZWNLFWQPQCGZSF-UHFFFAOYSA-N
Formula:	C18H15BF6O4
SMILES:	COc1ccccc1OCC1COB(c2cc(C(F)(F)F)cc(C(F)(F)F)c2)O1
Mol. weight [g/mol]:	420.11

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.20		Crippen Method
logp	3.922		Crippen Method
rinpol	2081.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R146711&Units=SI

Legend

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

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