Benzoic acid, 2-(8'-trifluoromethyl-4'-quinolylamino)-, 2,3-dihydroxypropyl ester

Other names:	Floctafenine
	Benzoic acid, 2-[[8-(trifluoromethyl)-4-quinolinyl]amino]-, 2,3-dihydroxypropyl ester
	4-(o-(2',3'-Dihydroxypropyloxycarbonyl)phenyl)-amino-8-trifluoromethylquinoline
	2,3-Dihydroxypropyl N-(8-(trifluoromethyl)-4-quinolyl)anthranilate
	Diralgan
	Idarac
	Novodolan
	R 4318
	RU 15750
	8-Trifluoromethyl-7-deschloroglafenine
	2-(8'-Trifluoromethyl-4'-quinolylamino)benzoic acid 2,3-dihydroxy propyl ester
	Idalon
	R-4138
Inchi:	InChI=1S/C20H17F3N2O4/c21-20(22,23)15-6-3-5-13-17(8-9-24-18(13)15)25-16-7-2-1-4-
InchiKey:	APQPGQGAWABJLN-UHFFFAOYSA-N
Formula:	C20H17F3N2O4
SMILES:	O=C(OCC(O)CO)c1ccccc1Nc1ccnc2c(C(F)(F)F)cccc12
Mol. weight [g/mol]:	406.36
CAS:	23779-99-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.67		Crippen Method
logp	3.507		Crippen Method
mcvol	270.130	ml/mol	McGowan Method
rinpol	3132.00		NIST Webbook
rinpol	3132.00		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=C23779999&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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