trans-3-Trifluoromethylcinnamic acid, morpholide

Inchi: InChI=1S/C14H14F3NO2/c15-14(16,17)12-3-1-2-11(10-12)4-5-13(19)18-6-8-20-9-7-18/h
InchiKey: WPNBCMAJDAVTKX-SNAWJCMRSA-N
Formula: C14H14F3NO2
SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)N1CCOCC1
Mol. weight [g/mol]: 285.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Crippen Method
logp	2.577		Crippen Method
mcvol	191.930	ml/mol	McGowan Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		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=U307366&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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