4-Trifluoromethylbenzoic acid, morpholide

Inchi: InChI=1S/C12H12F3NO2/c13-12(14,15)10-3-1-9(2-4-10)11(17)16-5-7-18-8-6-16/h1-4H,5
InchiKey: MYRLQCZKMYLLEM-UHFFFAOYSA-N
Formula: C12H12F3NO2
SMILES: O=C(c1ccc(C(F)(F)F)cc1)N1CCOCC1
Mol. weight [g/mol]: 259.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.178		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307244&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.