Pentafluorobenzoic acid, morpholide

Inchi: InChI=1S/C11H8F5NO2/c12-6-5(7(13)9(15)10(16)8(6)14)11(18)17-1-3-19-4-2-17/h1-4H2
InchiKey: DDWJJZXYZPMXLQ-UHFFFAOYSA-N
Formula: C11H8F5NO2
SMILES: O=C(c1c(F)c(F)c(F)c(F)c1F)N1CCOCC1
Mol. weight [g/mol]: 281.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	1.855		Crippen Method
mcvol	157.500	ml/mol	McGowan Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		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=U307373&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

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