1-Phenyl-2-pyrazyl-tetrafluoroethane

Inchi: InChI=1S/C12H8F4N2/c13-11(14,9-4-2-1-3-5-9)12(15,16)10-8-17-6-7-18-10/h1-8H
InchiKey: VOHULKRTQBHUJI-UHFFFAOYSA-N
Formula: C12H8F4N2
SMILES: FC(F)(c1ccccc1)C(F)(F)c1cnccn1
Mol. weight [g/mol]: 256.20
CAS: 116403-10-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.360		Crippen Method
mcvol	159.460	ml/mol	McGowan Method

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=C116403102&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