1,3-Bis(2-phenyl-1,3,4-oxadiazol-5-yl)perfluoropro

Inchi: InChI=1S/C19H10F6N4O2/c20-17(21,15-28-26-13(30-15)11-7-3-1-4-8-11)19(24,25)18(2
InchiKey: MMABQVGOFGJOQC-UHFFFAOYSA-N
Formula: C19H10F6N4O2
SMILES: FC(F)(c1nnc(-c2ccccc2)o1)C(F)(F)C(F)(F)c1nnc(-c2ccccc2)o1
Mol. weight [g/mol]: 440.30
CAS: 5086-79-3

Physical Properties

Property code	Value	Unit	Source
ie	9.50 ± 0.10	eV	NIST Webbook
log10ws	-17.10		Crippen Method
logp	5.306		Crippen Method
mcvol	254.410	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=C5086793&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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