2-Perfluoropropyl-5-phenyl-1,3,4-oxadiazole

Inchi: InChI=1S/C11H5F7N2O/c12-9(13,10(14,15)11(16,17)18)8-20-19-7(21-8)6-4-2-1-3-5-6/h1
InchiKey: ITYOBZDILJDFMZ-UHFFFAOYSA-N
Formula: C11H5F7N2O
SMILES: FC(F)(F)C(F)(F)C(F)(F)c1nnc(-c2ccccc2)o1
Mol. weight [g/mol]: 314.16
CAS: 5756-67-2

Physical Properties

Property code	Value	Unit	Source
ie	9.80 ± 0.20	eV	NIST Webbook
log10ws	-9.91		Crippen Method
logp	4.026		Crippen Method
mcvol	160.850	ml/mol	McGowan Method

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=C5756672&Units=SI

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.