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

Inchi: InChI=1S/C15H5F15N2O/c16-9(17,8-32-31-7(33-8)6-4-2-1-3-5-6)10(18,19)11(20,21)12(2
InchiKey: YNHVEOXJDBDTKS-UHFFFAOYSA-N
Formula: C15H5F15N2O
SMILES: FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)c1nnc(-c2ccccc2)o1
Mol. weight [g/mol]: 514.19
CAS: 5756-55-8

Physical Properties

Property code	Value	Unit	Source
ie	9.90 ± 0.10	eV	NIST Webbook
log10ws	-12.84		Crippen Method
logp	6.567		Crippen Method
mcvol	231.370	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=C5756558&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.