

Picolinafen

Inchi: InChI=1S/C19H12F4N2O2/c20-13-7-9-14(10-8-13)24-18(26)16-5-2-6-17(25-16)27-15-4-3
InchiKey: CWKFPEBMTGKCLKX-UHFFFAOYSA-N
Formula: C19H12F4N2O2
SMILES: O=C(Nc1ccc(F)cc1)c1cccc(Oc2cccc(C(F)(F)F)c2)n1
Mol. weight [g/mol]: 376.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	5.284		Crippen Method
mcvol	241.770	ml/mol	McGowan Method
rinpol	2483.00		NIST Webbook
rinpol	2477.00		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=R566239&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

Latest version available from:

<https://www.chemeo.com/cid/35-229-9/Picolinafen.pdf>

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