3,5-Difluoromethylbenzylamine, N-(4-pyridyl)methylene-

Inchi: InChI=1S/C15H10F6N2/c16-14(17,18)12-5-11(6-13(7-12)15(19,20)21)9-23-8-10-1-3-22-4

InchiKey: MYBPPYMAKYKVLW-UHFFFAOYSA-N

Formula: C15H10F6N2

SMILES: FC(F)(F)c1cc(CN=Cc2ccncc2)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 332.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.62		Crippen Method
logp	4.738		Crippen Method
mcvol	200.970	ml/mol	McGowan Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		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=U376708&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

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