Inabenfide

Other names: 4-Pyridinecarboxamide, N-[4-chloro-2-(hydroxyphenylmethyl)phenyl]-
Inchi: InChI=1S/C19H15ClN2O2/c20-15-6-7-17(22-19(24)14-8-10-21-11-9-14)16(12-15)18(23)
InchiKey: PFDCOZXELJAUTR-UHFFFAOYSA-N
Formula: C19H15ClN2O2
SMILES: O=C(Nc1ccc(Cl)cc1C(O)c1ccccc1)c1ccncc1
Mol. weight [g/mol]: 338.79

Physical Properties

Property code	Value	Unit	Source
logp	4.069		Crippen Method
mcvol	246.930	ml/mol	McGowan Method
rinpol	3108.70		NIST Webbook
rinpol	3108.70		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C82211243&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/91-818-3/Inabenfide.pdf

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