

(.+/-)-Isoboldine

Inchi: InChI=1S/C19H21NO4/c1-20-5-4-10-8-16(24-3)19(22)18-12-9-15(23-2)14(21)7-11(12)6-
InchiKey: LINHZVMHXABQLB-UHFFFAOYSA-N
Formula: C19H21NO4
SMILES: COc1cc2c(cc1O)CC1c3c(cc(OC)c(O)c3-2)CCN1C
Mol. weight [g/mol]: 327.37
CAS: 5164-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Crippen Method
logp	2.867		Crippen Method
mcvol	242.790	ml/mol	McGowan Method
rinpola	3135.30		NIST Webbook
rinpola	3135.30		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5164932&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/96-379-6/Isoboldine.pdf>

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