

(R)-1,2-Dimethoxy-6-methyl-5,6,6a,7-tetrahydro-4H

Inchi: InChI=1S/C19H21NO2/c1-20-9-8-13-11-16(21-2)19(22-3)18-14-7-5-4-6-12(14)10-15(20)
InchiKey: ORJVQPIHKOARKV-OAHLLOKOSA-N
Formula: C19H21NO2
SMILES: COc1cc2c3c(c1OC)-c1cccc1CC3N(C)CC2
Mol. weight [g/mol]: 295.38
CAS: 475-83-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	3.456		Crippen Method
mcvol	231.050	ml/mol	McGowan Method
rinpola	2493.70		NIST Webbook
rinpola	2493.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C475832&Units=SI>
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>

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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