

6,7-Dimethoxy-2-(4-methoxyphenethyl)-4H-chrom

Inchi: InChI=1S/C20H20O5/c1-22-14-7-4-13(5-8-14)6-9-15-10-17(21)16-11-19(23-2)20(24-3)12
InchiKey: WYSWREVQEJRZIQ-UHFFFAOYSA-N
Formula: C20H20O5
SMILES: COc1ccc(CCc2cc(=O)c3cc(OC)c(OC)cc3o2)cc1
Mol. weight [g/mol]: 340.37
CAS: 117596-92-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.21		Crippen Method
logp	3.604		Crippen Method
mcvol	255.030	ml/mol	McGowan Method
rinpol	3145.30		NIST Webbook
rinpol	3145.30		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C117596926&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpol: Non-polar retention indices

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