

6-Methoxy-2-phenethyl-4H-chromen-4-one

Inchi: InChI=1S/C18H16O3/c1-20-14-9-10-18-16(11-14)17(19)12-15(21-18)8-7-13-5-3-2-4-6-13
InchiKey: JOYYVGVYUHRBAE-UHFFFAOYSA-N
Formula: C18H16O3
SMILES: COc1ccc2oc(CCc3ccccc3)cc(=O)c2c1
Mol. weight [g/mol]: 280.32
CAS: 84294-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.97		Crippen Method
logp	3.587		Crippen Method
mcvol	215.110	ml/mol	McGowan Method
rinpol	2613.20		NIST Webbook
rinpol	2613.20		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C84294893&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

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