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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84294893&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
rinpol:	Non-polar retention indices

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