2-Phenethyl-4H-chromen-4-one

Other names:	Flidersiachromone
	Flindersiachromone
	2-(2-Phenylethyl)chromone
	4H-1-Benzopyran-4-one, 2-(2-phenylethyl)-
	Chromone, 2-(2-phenylethyl)
Inchi:	InChI=1S/C17H14O2/c18-16-12-14(11-10-13-6-2-1-3-7-13)19-17-9-5-4-8-15(16)17/h1-9,
InchiKey:	VNZNWFQJBFLELF-UHFFFAOYSA-N
Formula:	C17H14O2
SMILES:	O=c1cc(CCc2ccccc2)oc2ccccc12
Mol. weight [g/mol]:	250.29
CAS:	61828-53-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.85		Crippen Method
logp	3.578		Crippen Method
mcvol	195.150	ml/mol	McGowan Method
rinpol	2346.40		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2346.40		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61828533&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