

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

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