

Chromone, 6-methoxy-2-[2-(4-methoxyphenyl)ethyl]

Inchi:	InChI=1S/C19H18O4/c1-21-14-6-3-13(4-7-14)5-8-16-12-18(20)17-11-15(22-2)9-10-19(17-18)
InchiKey:	RQDQHEBGEUXELB-UHFFFAOYSA-N
Formula:	C19H18O4
SMILES:	COc1ccc(CCc2cc(=O)c3cc(OC)ccc3o2)cc1
Mol. weight [g/mol]:	310.34
CAS:	111286-05-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.09		Crippen Method
logp	3.595		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
rinpol	2926.40		NIST Webbook
rinpol	2926.40		NIST Webbook
rinpol	2949.00		NIST Webbook
rinpol	2949.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111286056&Units=SI
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

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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