2-(4-Methoxyphenethyl)-4H-chromen-4-one

Other names:	4H-1-Benzopyran-4-one, 2-[2-(4-methoxyphenyl)ethyl]-
	2-[2-(4-Methoxyphenyl)ethyl]chromone
	Chromone, 2-[2-(4-methoxyphenyl)ethyl]
Inchi:	InChI=1S/C18H16O3/c1-20-14-9-6-13(7-10-14)8-11-15-12-17(19)16-4-2-3-5-18(16)21-15
InchiKey:	ZQBJPQZBIGVILA-UHFFFAOYSA-N
Formula:	C18H16O3
SMILES:	COc1ccc(CCc2cc(=O)c3ccccc3o2)cc1
Mol. weight [g/mol]:	280.32
CAS:	92911-82-5

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	2545.00		NIST Webbook
rinpol	2545.00		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=C92911825&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