Elsholtzia ketone

Other names:	Dihydronaginata ketone
	Elsholtzione
	Elscholtzia ketone
Inchi:	InChI=1S/C10H14O2/c1-7(2)6-9(11)10-8(3)4-5-12-10/h4-5,7H,6H2,1-3H3
InchiKey:	MYPGRLGQLDFZMK-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	Cc1ccoc1C(=O)CC(C)C
Mol. weight [g/mol]:	166.22
CAS:	488-05-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.36		Crippen Method
logp	2.817		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1178.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1178.00		NIST Webbook

Sources

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=C488051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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