Perillaketone

Inchi: InChI=1S/C10H14O2/c1-8(2)3-4-10(11)9-5-6-12-7-9/h5-8H,3-4H2,1-2H3
InchiKey: LVHLZMUFIYAEQB-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(C)CCC(=O)c1ccoc1
Mol. weight [g/mol]: 166.22
CAS: 553-84-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.30		Crippen Method
logp	2.898		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
rinpol	1249.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1248.00		NIST Webbook
ripol	1811.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C553844&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices