Dehydroelsholtzia ketone

Inchi: InChI=1S/C10H12O2/c1-7(2)6-9(11)10-8(3)4-5-12-10/h4-6H,1-3H3
InchiKey: XWFVDCOWPBJQFH-UHFFFAOYSA-N
Formula: C10H12O2
SMILES: CC(C)=CC(=O)c1occc1C
Mol. weight [g/mol]: 164.20
CAS: 6138-88-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	2.737		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
rinpol	1287.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1306.10		NIST Webbook
rinpol	1298.00		NIST Webbook
ripol	1884.00		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=C6138881&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

ripol: Polar retention indices