Carr's ketol, TMS

Inchi: InChI=1S/C15H22O3/c1-10(2)8-13(16)14-11(3)4-6-15(14,17)12-5-7-18-9-12/h5,7,9-11,14
InchiKey: PLJLLELLRWAYEB-NILFDRSVSA-N
Formula: C15H22O3
SMILES: CC(C)CC(=O)C1C(C)CCC1(O)c1ccoc1
Mol. weight [g/mol]: 250.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.66		Crippen Method
logp	3.129		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
rinpol	1764.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R584806&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