(R,5E,9E)-8-Methoxy-3,6,10-trimethyl-4,7,8,11-tetra

Inchi: InChI=1S/C16H22O2/c1-11-5-6-15-13(3)10-18-16(15)9-12(2)8-14(7-11)17-4/h5,8,10,14H
InchiKey: NWLNPDFDTSFGEU-NJNKKQILSA-N
Formula: C16H22O2
SMILES: COC1C=C(C)Cc2occ(C)c2CC=C(C)C1
Mol. weight [g/mol]: 246.34
CAS: 108376-98-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.02		Crippen Method
logp	3.984		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
rinpol	1733.70		NIST Webbook
rinpol	1733.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C108376983&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