Euparin

Inchi: InChI=1S/C13H12O3/c1-7(2)12-5-9-4-10(8(3)14)11(15)6-13(9)16-12/h4-6,15H,1H2,2-3H
InchiKey: OPUFDNZTKHPZHM-UHFFFAOYSA-N
Formula: C13H12O3
SMILES: C=C(C)c1cc2cc(C(C)=O)c(O)cc2o1
Mol. weight [g/mol]: 216.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	3.374		Crippen Method
mcvol	164.120	ml/mol	McGowan Method
rinpol	1858.00		NIST Webbook
ripol	2797.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R518215&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