2-Benzofuranylethylene glycol

Inchi: InChI=1S/C10H10O3/c11-6-8(12)10-5-7-3-1-2-4-9(7)13-10/h1-5,8,11-12H,6H2
InchiKey: LRTYEGVIFGIVRB-UHFFFAOYSA-N
Formula: C10H10O3
SMILES: OCC(O)c1cc2ccccc2o1
Mol. weight [g/mol]: 178.18
CAS: 116346-32-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.80		Crippen Method
logp	1.458		Crippen Method
mcvol	130.450	ml/mol	McGowan Method

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=C116346328&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