

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

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<https://www.chemeo.com/cid/94-430-0/2-Benzofuranylethylene-glycol.pdf>

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