

6H-Dibenzo(b,d)pyran-6-one

Inchi: InChI=1S/C13H8O2/c14-13-11-7-2-1-5-9(11)10-6-3-4-8-12(10)15-13/h1-8H
InchiKey: TVKNXKLYVUVOCV-UHFFFAOYSA-N
Formula: C13H8O2
SMILES: O=c1oc2ccccc2c2ccccc12
Mol. weight [g/mol]: 196.20
CAS: 2005-10-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.24		Crippen Method
logp	2.946		Crippen Method
mcvol	143.090	ml/mol	McGowan Method
rinsol	325.87		NIST Webbook
tf	369.00 ± 2.00	K	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2005109&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinsol: Non-polar retention indices
tf: Normal melting (fusion) point

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