

Furan, 2,2'-methylenebis[5-methyl-

Other names: Furan, 2,2'-methylenebis*5-methyl-
Inchi: InChI=1S/C11H12O2/c1-8-3-5-10(12-8)7-11-6-4-9(2)13-11/h3-6H,7H2,1-2H3
InchiKey: FVKCJDISKKFSJI-UHFFFAOYSA-N
Formula: C11H12O2
SMILES: Cc1ccc(Cc2ccc(C)o2)o1
Mol. weight [g/mol]: 176.21
CAS: 13679-43-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.99		Crippen Method
logp	3.080		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
ripol	1732.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1729.00		NIST Webbook
ripol	1731.00		NIST Webbook
ripol	1731.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13679431&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

ripol: Polar retention indices

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