

1,3-Benzodioxol-2-one, 5-(1,1-dimethylethyl)-

Other names:	5-Tert-butyl-1,3-benzodioxol-2-one
Inchi:	InChI=1S/C11H12O3/c1-11(2,3)7-4-5-8-9(6-7)14-10(12)13-8/h4-6H,1-3H3
InchiKey:	KLQJKXDFHGURBO-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	CC(C)(C)c1ccc2oc(=O)oc2c1
Mol. weight [g/mol]:	192.21
CAS:	54815-21-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.48		Crippen Method
logp	2.683		Crippen Method
mcvol	144.540	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54815213&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

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