Furan, 2,5-dibutyl-

Other names: 2,5-Dibutylfuran
Inchi: InChI=1S/C12H20O/c1-3-5-7-11-9-10-12(13-11)8-6-4-2/h9-10H,3-8H2,1-2H3
InchiKey: XTBSCDXJHDVPLX-UHFFFAOYSA-N
Formula: C12H20O
SMILES: CCCCc1ccc(CCCC)o1
Mol. weight [g/mol]: 180.29
CAS: 72636-53-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.49		Crippen Method
logp	3.965		Crippen Method
mcvol	166.350	ml/mol	McGowan Method
rinpol	1510.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72636534&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices