

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
rinpola	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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/52-150-7/Furan-2-5-dibutyl.pdf>

Generated by Cheméo on 2024-04-20 04:35:17.445219205 +0000 UTC m=+15876966.365796520.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.