

Furan, 2-(1,1-dimethylethyl)-4-methyl-

Other names:	Furan, 2-tert-butyl-4-methyl- 2-tert-Butyl-4-methylfuran
Inchi:	InChI=1S/C9H14O/c1-7-5-8(10-6-7)9(2,3)4/h5-6H,1-4H3
InchiKey:	DDXRLYGFNHYHBOK-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	<chem>Cc1coc(C(C)(C)C)c1</chem>
Mol. weight [g/mol]:	138.21
CAS:	6141-68-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.99		Crippen Method
logp	2.886		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
tb	419.65 ± 1.00	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6141680&Units=SI

Legend

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

tb: Normal Boiling Point Temperature

Latest version available from:

<https://www.cheméo.com/cid/21-072-8/Furan-2-1-1-dimethylethyl-4-methyl.pdf>

Generated by Cheméo on 2024-04-20 04:16:00.956201589 +0000 UTC m=+15875809.876778905.

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