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: DDXRLYGFNYHBOK-UHFFFAOYSA-N
Formula: C9H14O
SMILES: Cc1coc(C(C)(C)C)c1
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/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=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