

1,2,3,4-Tetrahydrodibenzofuran

Other names:	Dibenzofuran, 1,2,3,4-tetrahydro-
Inchi:	InChI=1S/C12H12O/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1,3,5,7H,2,4,6,8H2
InchiKey:	LREHXNMBUBVFHA-UHFFFAOYSA-N
Formula:	C12H12O
SMILES:	<chem>c1ccc2c3c(oc2c1)CCCC3</chem>
Mol. weight [g/mol]:	172.22
CAS:	13130-19-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.51		Crippen Method
logp	3.312		Crippen Method
mcvol	136.030	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.50 ± 0.50	K	2.00	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=C13130193&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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