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: c1ccc2c3c(oc2c1)CCCC3
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/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=C13130193&Units=SI

Legend

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