

2-Benzofurancarboxaldehyde, 3-methyl-

Inchi: InChI=1S/C10H8O2/c1-7-8-4-2-3-5-9(8)12-10(7)6-11/h2-6H,1H3
InchiKey: UBJKHRKGYBTDIA-UHFFFAOYSA-N
Formula: C10H8O2
SMILES: Cc1c(C=O)oc2ccccc12
Mol. weight [g/mol]: 160.17
CAS: 1199-07-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.73		Crippen Method
logp	2.554		Crippen Method
mcvol	120.280	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1199071&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/41-164-4/2-Benzofurancarboxaldehyde-3-methyl.pdf>

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