

Ethyl 5-benzyloxyindole-2-carboxylate

Other names:

5-Benzyloxyindole-2-carboxylic acid ethylester
1H-Indole-2-carboxylic acid, 5-(phenylmethoxy)-, ethyl ester
ethyl 5-(phenylmethoxy)-1H-indole-2-carboxylate

Inchi:

InChI=1S/C18H17NO3/c1-2-21-18(20)17-11-14-10-15(8-9-16(14)19-17)22-12-13-6-4-3-5

InchiKey:

DCIFXYFKVKDOLL-UHFFFAOYSA-N

Formula:

C18H17NO3

SMILES:

CCOC(=O)c1cc2cc(OCc3ccccc3)ccc2[nH]1

Mol. weight [g/mol]:

295.33

CAS:

37033-95-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	3.442		Crippen Method
mcvol	225.090	ml/mol	McGowan Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C37033957&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

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<https://www.chemeo.com/cid/99-291-0/Ethyl-5-benzyloxyindole-2-carboxylate.pdf>

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