

DL-Tryptophan, N-acetyl-

Other names:

Tryptophan, N-acetyl-, DL-
DL-«alpha»-Acetylamino-3-indolepropionic acid
DL-Acetyltryptophan
DL-N-Acetyltryptophan
N-Acetyl-DL-tryptophan
N-Acetyl-DL-tryptophane
dl-«alpha»-Acetamidoindole-3-propionic acid
Acetyl-DL-tryptophan
NSC 49124
Tryptophan, N-acetyl-
N«alpha»-acetyl-DL-tryptophan

Inchi:

InChI=1S/C13H14N2O3/c1-8(16)15-12(13(17)18)6-9-7-14-11-5-3-2-4-10(9)11/h2-5,7,12,

InchiKey:

DZTHIGRZJZPRDV-UHFFFAOYSA-N

Formula:

C13H14N2O3

SMILES:

CC(=O)NC(Cc1c[nH]c2ccccc12)C(=O)O

Mol. weight [g/mol]:

246.26

CAS:

87-32-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	0.818		Crippen Method
mcpvol	184.080	ml/mol	McGowan Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C87321&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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