

Propyliodone

Other names:

1(4H)-Pyridineacetic acid, 3,5-diiodo-4-oxo-, propyl ester
A. G. 33-107
Bronchodiagnostin
Bronkhodiagnostin
Brosombra
Dionosil
Diostril
Propiodone
Propyl 3,5-diiodo-4-pyridone-N-acetate
Propyl-3,5-diiodo-4-oxo-1(4H)pyridine, acetate
Propyliodon
3,5-Diiodo-4-oxo-1(4H)-pyridineacetic acid propyl ester
3,5-Diiodo-4-pyridone-N-acetic acid propyl ester
3,5-Diiodo-1-propoxycarbonylmethylpyrid-4-one
Pyridine acetic acid, 3,5-diiodo-4-oxo-1(4H)-, propyl ester
NSC 97103

Inchi:

InChI=1S/C10H11I2NO3/c1-2-3-16-9(14)6-13-4-7(11)10(15)8(12)5-13/h4-5H,2-3,6H2,1H

InchiKey:

ROSXARVHJNYYDO-UHFFFAOYSA-N

Formula:

C10H11I2NO3

SMILES:

CCCOC(=O)Cn1cc(I)c(=O)c(I)c1

Mol. weight [g/mol]:

447.01

CAS:

587-61-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	2.011		Crippen Method
mvol	202.930	ml/mol	McGowan Method

Sources

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=C587611&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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.cheméo.com/cid/46-275-6/Propylidone.pdf>

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