

Isonipecotic acid, N-(bromoacetyl)-, hexyl ester

Inchi:	InChI=1S/C14H24BrNO3/c1-2-3-4-5-10-19-14(18)12-6-8-16(9-7-12)13(17)11-15/h12H,2-
InchiKey:	ULURFYYPVQTOS-UHFFFAOYSA-N
Formula:	C14H24BrNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)CBr)CC1
Mol. weight [g/mol]:	334.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	2.743		Crippen Method
mcvol	233.750	ml/mol	McGowan Method
rinpole	2406.00		NIST Webbook
rinpole	2406.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361535&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/115-104-8/Isonipecotic-acid-N-bromoacetyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-28 19:58:07.435373482 +0000 UTC m=+16623536.355950793.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.