

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

Inchi:	InChI=1S/C14H24BrNO3/c1-11(2)4-3-9-19-14(18)12-5-7-16(8-6-12)13(17)10-15/h11-12H
InchiKey:	BMVGROMDEPEEQJ-UHFFFAOYSA-N
Formula:	C14H24BrNO3
SMILES:	CC(C)CCOC(=O)C1CCN(C(=O)CBr)CC1
Mol. weight [g/mol]:	334.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	2.599		Crippen Method
mcvol	233.750	ml/mol	McGowan Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook

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=U361534&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
rinpol:	Non-polar retention indices

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