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

Inchi: InChI=1S/C17H30BrNO3/c1-2-3-4-5-6-7-8-13-22-17(21)15-9-11-19(12-10-15)16(20)14-1

InchiKey: IADFLLOBXZRSGR-UHFFFAOYSA-N

Formula: C17H30BrNO3

SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)CBr)CC1

Mol. weight [g/mol]: 376.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.914		Crippen Method
mcvol	276.020	ml/mol	McGowan Method
rinpol	2722.00		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=U361538&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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