

# Isonipectic 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
rinpole	2722.00		NIST Webbook

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361538&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361538&amp;Units=SI</a>

## Legend

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

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