

# 2-Furamidoxime, o-(2-bromobutyryl)-5-nitro-

<b>Inchi:</b>	InChI=1S/C9H10BrN3O5/c1-2-5(10)9(14)18-12-8(11)6-3-4-7(17-6)13(15)16/h3-5H,2H2,1
<b>InchiKey:</b>	QBNSKOTYFBIIDI-UHFFFAOYSA-N
<b>Formula:</b>	C9H10BrN3O5
<b>SMILES:</b>	CCC(Br)C(=O)ON=C(N)c1ccc([N+](=O)[O-])o1
<b>Mol. weight [g/mol]:</b>	320.10

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.51		Crippen Method
logp	1.525		Crippen Method
mcvol	182.100	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009045&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009045&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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