

# Pipobroman

<b>Other names:</b>	A 1803 A-8103 Amedel N,N'-Bis(3-bromopropionyl)piperazine NSC-25154 Piperazine, 1,4-bis(3-bromo-1-oxopropyl)- Piperazine, 1,4-bis(3-bromopropionyl)- Vercyte 1,4-Bis(3-bromopropionyl)piperazine N,N-Bis-(3-bromopropionyl)-piperazine
<b>Inchi:</b>	InChI=1S/C10H16Br2N2O2/c11-3-1-9(15)13-5-7-14(8-6-13)10(16)2-4-12/h1-8H2
<b>InchiKey:</b>	NJBFOOCLYDNZJN-UHFFFAOYSA-N
<b>Formula:</b>	C10H16Br2N2O2
<b>SMILES:</b>	O=C(CCBBr)N1CCN(C(=O)CCBr)CC1
<b>Mol. weight [g/mol]:</b>	356.05
<b>CAS:</b>	54-91-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	1.227		Crippen Method
mcvol	199.000	ml/mol	McGowan Method
rinpola	2030.00		NIST Webbook
rinpola	2050.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54911&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54911&amp;Units=SI</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
<b>rinpol:</b>	Non-polar retention indices

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