Pipobroman

Other names:	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
Inchi:	InChI=1S/C10H16Br2N2O2/c11-3-1-9(15)13-5-7-14(8-6-13)10(16)2-4-12/h1-8H2
InchiKey:	NJBFOOCLYDNZJN-UHFFFAOYSA-N
Formula:	C10H16Br2N2O2
SMILES:	O=C(CCBr)N1CCN(C(=O)CCBr)CC1
Mol. weight [g/mol]:	356.05
CAS:	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
rinpol	2030.00		NIST Webbook
rinpol	2050.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C54911&Units=SI

Legend

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