

1H-Isoindole-1,3(2H)-dione, 2-(4-bromobutyl)-

Other names:	N-(4-Bromobutyl)phthalimide 4-Bromobutylphthalimide Phthalimide, N-(4-bromobutyl)- 1-Phthalimido-4-bromobutane N-(«omega»-Bromobutyl)phthalimide
Inchi:	InChI=1S/C12H12BrNO2/c13-7-3-4-8-14-11(15)9-5-1-2-6-10(9)12(14)16/h1-2,5-6H,3-4,7
InchiKey:	UXFWTIGUWHJKDD-UHFFFAOYSA-N
Formula:	C12H12BrNO2
SMILES:	O=C1c2cccc2C(=O)N1CCCCBr
Mol. weight [g/mol]:	282.13
CAS:	5394-18-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.458		Crippen Method
mcvol	175.940	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5394183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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