

N-(8-Bromooctyl)phthalimide

Inchi:	InChI=1S/C16H20BrNO2/c17-11-7-3-1-2-4-8-12-18-15(19)13-9-5-6-10-14(13)16(18)20/h
InchiKey:	LAMUQORCSIHVMC-UHFFFAOYSA-N
Formula:	C16H20BrNO2
SMILES:	O=C1c2ccccc2C(=O)N1CCCCCCCCBr
Mol. weight [g/mol]:	338.24
CAS:	17702-83-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.018		Crippen Method
mcvol	232.300	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=C17702839&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

Latest version available from:

<https://www.chemeo.com/cid/123-173-3/N-8-Bromooctyl-phthalimide.pdf>

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