

1H-Isoindole-1,3(2H)-dione, 2-(3-bromopropyl)-

Other names:	N-(3-Bromopropyl)phthalimide N-(3-Bromo-1-propyl)phthalimide «gamma»-Bromopropylphthalimide 3-Bromopropylphthalimide Phthalimide, N-(3-bromopropyl)- 1-Phthalimido-3-bromopropane
Inchi:	InChI=1S/C11H10BrNO2/c12-6-3-7-13-10(14)8-4-1-2-5-9(8)11(13)15/h1-2,4-5H,3,6-7H2
InchiKey:	VKJJCJJYNVIYVQR-UHFFFAOYSA-N
Formula:	C11H10BrNO2
SMILES:	O=C1c2ccccc2C(=O)N1CCCB
Mol. weight [g/mol]:	268.11
CAS:	5460-29-7

Physical Properties

Property code	Value	Unit	Source
hsub	116.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-3.10		Crippen Method
logp	2.068		Crippen Method
mvol	161.850	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=C5460297&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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