N-(4-bromobutyl)phthalimide

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=C1c2ccccc2C(=O)N1CCCCBr
Mol. weight [g/mol]:	282.14

Physical Properties

Property code	Value	Unit	Source
hf	-260.17	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
logp	2.458		Crippen Method
mcvol	175.940	ml/mol	McGowan Method
tb	634.81	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5394183&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature