N-(2-Bromopropyl)phthalimide

Other names: N-(2-Bromopropyl)phthalimide
Inchi: InChI=1S/C11H10BrNO2/c1-7(12)6-13-10(14)8-4-2-3-5-9(8)11(13)15/h2-5,7H,6H2,1H3
InchiKey: OEDMJTQRHMQBHD-UHFFFAOYSA-N
Formula: C11H10BrNO2
SMILES: CC(Br)CN1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 268.11

Physical Properties

Property code	Value	Unit	Source
hf	-245.33	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
logp	2.066		Crippen Method
mcvol	161.850	ml/mol	McGowan Method
tb	618.80	K	Cheméo Relay (1.0)
tf	400.41	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21134258&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

tf: Normal melting (fusion) point