2-Bromobenzoic acid, morpholide

Inchi: InChI=1S/C11H12BrNO2/c12-10-4-2-1-3-9(10)11(14)13-5-7-15-8-6-13/h1-4H,5-8H2
InchiKey: QPQCGIYRAMNHKH-UHFFFAOYSA-N
Formula: C11H12BrNO2
SMILES: O=C(c1ccccc1Br)N1CCOCC1
Mol. weight [g/mol]: 270.12

Physical Properties

Property code	Value	Unit	Source
hf	-187.30	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-1.86		Cheméo Relay (1.0)
logp	1.921		Crippen Method
mcvol	166.150	ml/mol	McGowan Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	628.36	K	Cheméo Relay (1.0)
tf	330.53	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307382&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

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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