3-Bromobenzoic acid, morpholide

Inchi: InChI=1S/C11H12BrNO2/c12-10-3-1-2-9(8-10)11(14)13-4-6-15-7-5-13/h1-3,8H,4-7H2
InchiKey: ZVHMYYPSUJGLHH-UHFFFAOYSA-N
Formula: C11H12BrNO2
SMILES: O=C(c1cccc(Br)c1)N1CCOCC1
Mol. weight [g/mol]: 270.12

Physical Properties

Property code	Value	Unit	Source
hf	-192.91	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-2.13		Cheméo Relay (1.0)
logp	1.921		Crippen Method
mcvol	166.150	ml/mol	McGowan Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	627.40	K	Cheméo Relay (1.0)
tf	320.13	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307150&Units=SI

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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