L-Proline, N-(4-bromobenzoyl)-, methyl ester

Inchi: InChI=1S/C13H14BrNO3/c1-18-13(17)11-3-2-8-15(11)12(16)9-4-6-10(14)7-5-9/h4-7,11H
InchiKey: HNEKOXRDLTYVBE-UHFFFAOYSA-N
Formula: C13H14BrNO3
SMILES: COC(=O)C1CCCN1C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 312.16

Physical Properties

Property code	Value	Unit	Source
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-3.22		Cheméo Relay (1.0)
logp	2.227		Crippen Method
mcvol	195.900	ml/mol	McGowan Method
rinpol	2170.00		NIST Webbook
tf	363.98	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299616&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):
Cheméo Relay (1.0, beta):

Legend

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

tf: Normal melting (fusion) point