Thiophene-2-carboxamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C11H8BrNOS/c12-8-3-5-9(6-4-8)13-11(14)10-2-1-7-15-10/h1-7H,(H,13,14)
InchiKey: GOSYKGLEOORQPW-UHFFFAOYSA-N
Formula: C11H8BrNOS
SMILES: O=C(Nc1ccc(Br)cc1)c1cccs1
Mol. weight [g/mol]: 282.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	3.763		Crippen Method
mcvol	168.030	ml/mol	McGowan Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307072&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.