Acetamide, N-(4-bromophenyl)-2-(2-thienyl)-

Inchi: InChI=1S/C12H10BrNOS/c13-9-3-5-10(6-4-9)14-12(15)8-11-2-1-7-16-11/h1-7H,8H2,(H,1
InchiKey: IQPFTYHOJYZMRQ-UHFFFAOYSA-N
Formula: C12H10BrNOS
SMILES: O=C(Cc1cccs1)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 296.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.21		Crippen Method
logp	3.692		Crippen Method
mcvol	182.120	ml/mol	McGowan Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U306905&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.