

5-Bromopentanoic acid, morpholide

Inchi: InChI=1S/C9H16BrNO2/c10-4-2-1-3-9(12)11-5-7-13-8-6-11/h1-8H2
InchiKey: BKXCUDHMUGGCCN-UHFFFAOYSA-N
Formula: C9H16BrNO2
SMILES: O=C(CCCCBBr)N1CCOCC1
Mol. weight [g/mol]: 250.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	1.410		Crippen Method
mcvol	161.730	ml/mol	McGowan Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U306987&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

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