

Isonipecotic acid, N-(bromoacetyl)-, octyl ester

Inchi: InChI=1S/C16H28BrNO3/c1-2-3-4-5-6-7-12-21-16(20)14-8-10-18(11-9-14)15(19)13-17/h
InchiKey: MYVFEJSXUREHQO-UHFFFAOYSA-N
Formula: C16H28BrNO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)CBr)CC1
Mol. weight [g/mol]: 362.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	3.524		Crippen Method
mcvol	261.930	ml/mol	McGowan Method
rinpol	2620.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361537&Units=SI>

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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