

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

Inchi: InChI=1S/C10H16BrNO3/c1-2-15-10(14)8-3-5-12(6-4-8)9(13)7-11/h8H,2-7H2,1H3
InchiKey: KJOUBCZYBMZWNO-UHFFFAOYSA-N
Formula: C10H16BrNO3
SMILES: CCOC(=O)C1CCN(C(=O)CBr)CC1
Mol. weight [g/mol]: 278.14

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -1.30 | | Crippen Method |
| logp | 1.183 | | Crippen Method |
| mcvol | 177.390 | ml/mol | McGowan Method |
| rinpole | 1973.00 | | NIST Webbook |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361533&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

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