

1-(P-nitrobenzyl)-5-amyl-5-ethylbarbituric acid

Inchi: InChI=1S/C18H23N3O5/c1-3-5-6-11-18(4-2)15(22)19-17(24)20(16(18)23)12-13-7-9-14(1)
InchiKey: LQJFANKQMOSOLM-UHFFFAOYSA-N
Formula: C18H23N3O5
SMILES: CCCCC1(CC)C(=O)N(Cc2ccc([N+](=O)[O-])cc2)C(=O)N=C1O
Mol. weight [g/mol]: 361.39

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.34 | | Crippen Method |
| logp | 3.990 | | Crippen Method |
| mcvol | 271.950 | ml/mol | McGowan Method |

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=B6003514&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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