

3-Butanoyloxymethylphenytoin

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|-----------------------------|--|
| Other names: | [2,5-dioxo-4,4-di(phenyl)imidazolidin-1-yl]methyl butanoate |
| Inchi: | InChI=1S/C20H20N2O4/c1-2-9-17(23)26-14-22-18(24)20(21-19(22)25,15-10-5-3-6-11-15 |
| InchiKey: | UPQWMVAELITTGQ-UHFFFAOYSA-N |
| Formula: | C20H20N2O4 |
| SMILES: | CCCC(=O)OCN1C(=O)NC(c2ccccc2)(c2ccccc2)C1=O |
| Mol. weight [g/mol]: | 352.39 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| log10ws | -4.83 | | Aqueous Solubility Prediction Method |
| log10ws | -5.07 | | Estimated Solubility Method |
| logp | 2.783 | | Crippen Method |
| mcvol | 264.820 | ml/mol | McGowan Method |
| tf | 404.25 | K | Aqueous Solubility Prediction Method |

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| tf: | Normal melting (fusion) point |

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