2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-phenyl-1-(phenylmethyl)-

Other names: 1-Benzyl-5-phenylbarbituric acid
Inchi: InChI=1S/C17H14N2O3/c20-15-14(13-9-5-2-6-10-13)16(21)19(17(22)18-15)11-12-7-3-1-
InchiKey: KCWWCWMGJOWTMY-UHFFFAOYSA-N
Formula: C17H14N2O3
SMILES: O=C1NC(=O)N(Cc2ccccc2)C(=O)C1c1ccccc1
Mol. weight [g/mol]: 294.30
CAS: 72846-00-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.049		Crippen Method
mcvol	216.680	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72846005&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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