

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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/32-242-7/2-4-6-1H-3H-5H-Pyrimidinetrione-5-phenyl-1-phenylmethyl.pdf>

Generated by Cheméo on 2024-04-20 05:13:39.118554312 +0000 UTC m=+15879268.039131634.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.