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: CCCCCC1(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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003514&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