1,3-Di(p-nitrobenzyl)-5-amyl-5-ethylbarbituric acid

Inchi: InChI=1S/C25H28N4O7/c1-3-5-6-15-25(4-2)22(30)26(16-18-7-11-20(12-8-18)28(33)34)2

InchiKey: UKNKCRDQHXIVMZ-UHFFFAOYSA-N

Formula: C25H28N4O7

SMILES: CCCCCC1(CC)C(=O)N(Cc2ccc([N+](=O)[O-])cc2)C(=O)N(Cc2ccc([N+](=O)[O-])cc2)C1=

Mol. weight [g/mol]: 496.51

CAS: 116465-41-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.88		Crippen Method
logp	4.971		Crippen Method
mcvol	364.240	ml/mol	McGowan Method

Sources

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=C116465419&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume