

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:	CCCCC1(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

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