

Suxibuzone

Other names:	Butanedioic acid, mono[(4-butyl-3,5-dioxo-1,2-diphenyl-4-pyrazolidinyl)methyl] ester. Succinic acid, monoester with 4-butyl-4-(hydroxymethyl)-1,2-diphenyl-3,5-pyrazolidinedione 4-Butyl-4-(«beta»-carboxypropionyl-oxymethyl)-1,2-diphenyl-3,5-pyrazolidinedione 4-Butyl-4-hydroxymethyl-1,2-diphenyl-3,5-pyrazolidinedione hydrogen succinate 4-Butyl-4-(hydroxymethyl)-1,2-diphenyl-3,5-pyrazolidinedione hydrogen succinate (ester) AE-17 Danilon Flogos Solurol 4-[(4-Butyl-3,5-dioxo-1,2-diphenyl-4-pyrazolidinyl)methoxy]-4-oxobutanoic acid 3,5-Pyrazolidinedione, 4-butyl-4-(hydroxymethyl)-1,2-diphenyl-, hydrogen succinate (ester) 4-Hydroxymethylbutazolidine hemisuccinate Calibene
Inchi:	InChI=1S/C24H26N2O6/c1-2-3-16-24(17-32-21(29)15-14-20(27)28)22(30)25(18-10-6-4-7
InchiKey:	ONWXNHPOAGOMTG-UHFFFAOYSA-N
Formula:	C24H26N2O6
SMILES:	CCCCC1(COC(=O)CCC(=O)O)C(=O)N(c2ccccc2)N(c2ccccc2)C1=O
Mol. weight [g/mol]:	438.47
CAS:	27470-51-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.566		Crippen Method
mcvol	328.620	ml/mol	McGowan Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27470515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpol:	Non-polar retention indices

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