3,5-Pyrazolidinedione, 4-butyl-1-phenyl-

Other names:	3,5-Pyrazolidinedione, 4-butyl-1-phenyl-
	Arcobutine
	Butazone
	Mobutazon
	Mobutazone
	Mobuzon
	Monazan
	Monobutyl
	Monofen
	Monomil
	Monophenylbutazone
	Monorheumetten
	Monozon
	Mophebutazone
	Mozol
	Reumatox
	4-Butyl-3,5-diketo-1-phenylpyrazolidine
	Arcomonol tablets
	Corbuton
	4-Butyl-1-phenyl-3,5-dioxopyrazolidine
	4-Butyl-1-phenyl-3,5-pyrazolidinedione
	2 Fdbp
	Mofesal
	Monazon
	2-Phenyl-3,5-dihydroxy-4-butylpyrazolidine
	NSC 73725
	1-Phenyl-4-butyl-3,5-pyrazolidinedione
	4-Butyl-1-phenyl-pyrazolidine-3,5-dione
Inchi:	InChI=1S/C13H16N2O2/c1-2-3-9-11-12(16)14-15(13(11)17)10-7-5-4-6-8-10/h4-8,11H,2-3
InchiKey:	REOJLIXKJWXUGB-UHFFFAOYSA-N
Formula:	C13H16N2O2
SMILES:	CCCCC1C(=O)NN(c2ccccc2)C1=O
Mol. weight [g/mol]:	232.28

Physical Properties

Property code	Value	Unit	Source

log10ws	-2.98		Cheméo Relay (1.0)
logp	1.871		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
rinpol	2142.00		NIST Webbook
tf	431.18	K	Cheméo Relay (1.0)

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2210631&Units=SI

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

tf: Normal melting (fusion) point