

Sulfinpyrazone

Other names:

3,5-Pyrazolidinedione, 1,2-diphenyl-4-[2-(phenylsulfinyl)ethyl]-

Anturan

Anturane

Anturanil

Anturen

Anturidin

Diphenylpyrazone

Enturan

Enturen

G 28315

Sulfinpyrazine

Sulfinpyrazon

Sulfoxyphenylpyrazolidine

Sulphinpyrazone

USAF GE-13

1,2-Diphenyl-4-(2'-phenylsulfinethyl)-3,5-pyrazolidinedione

4-(Phenylsulfoxyethyl)-1,2-diphenyl-3,5-pyrazolidinedione

1,2-Diphenyl-3,5-dioxo-4-(2'-phenyl-sulfinyl-aethyl)-pyrazolidin

1,2-Diphenyl-4-[2-(phenylsulfinyl)ethyl]-3,5-pyrazolidinedione

Anturano

NSC 75925

Inchi:

InChI=1S/C23H20N2O3S/c26-22-21(16-17-29(28)20-14-8-3-9-15-20)23(27)25(19-12-6-2

InchiKey:

MBGGBVCUIVRRBF-UHFFFAOYSA-N

Formula:

C23H20N2O3S

SMILES:

O=C1C(CCS(=O)c2ccccc2)C(=O)N(c2ccccc2)N1c1ccccc1

Mol. weight [g/mol]:

404.48

CAS:

57-96-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.28		Crippen Method
logp	3.795		Crippen Method
mccvol	298.110	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57965&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

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