1H-Isoindole-1,3(2H)-dione, 2-(2,6-dioxo-3-piperidinyl)-

Other names:

(+/-)-Thalidomide
1,3-Dioxo-2-(2,6-dioxopiperidin-3-yl)isoindoline
2,6-Dioxo-3-phthalimidopiperidine
3-Phthalimidoglutarimide
Algosediv
Asidon 3
Asmadion
Asmaval
Bonbrain
Bonbrrin
Calmore
Calmorex
Celgene
Contergan
Corronarobetin
Distaval
Distaxal
Distoval
E-217
Ectiluran
Enterosediv
Gastrinide
Glupan
Glutanon
Glutarimide, 2-phthalimido-
Grippex
Hippuzon
Imida-Lab
Imidan (peyta)
Imidene
Isomin
K 17
Kedavon
Kevadon
Lulamin
N-(2,6-Dioxo-3-piperidyl)phthalimide
N-Phthaloylglutamimide
N-Phthalyl-glutaminsaeure-imid
N-Phthalylglutamic acid imide
NSC-66847

Neaufatin
Neo
Neosedyn
Neosydyn
Nerosedyn
Neufatin
Neurodyn
Neurosedin
Neurosedym
Neurosedyn
Nevrodyn
Nibrol
Noctosediv
Noxodyn
Pangul
Pantosediv
Pharmion
Phthalimide, N-(2,6-dioxo-3-piperidyl)-
Poly-Giron
Polygripan
Predni-Sediv
Pro-ban M
Profarmil
Psycholiquid
Psychotablets
Quetimid
Quietoplex
Sandormin
Sedalis
Sedalis sedi-lab
Sedimide
Sedin
Sedisperil
Sedoval
Shin-naito S
Shinnibrol
Sleepan
Slipro
Softenil
Softenon
Talargan
Talimol
Talinol

Talismol
Telagan
Telargan
Telargean
Tensival
Thalidomide
Thalin
Thalinette
Thalomid
Theophilcholine
Ulcerfen
Valgis
Valgraine
Yodomin
«alpha»-(N-Phthalimido)glutarimide
«alpha»-N-Phthalylglutaramide
«alpha»-Phthalimidoglutarimide
Â«alphaÂ»-(N-Phthalimido)glutarimide
Â«alphaÂ»-N-Phthalylglutaramide
Â«alphaÂ»-Phthalimidoglutarimide

Inchi: InChI=1S/C13H10N2O4/c16-10-6-5-9(11(17)14-10)15-12(18)7-3-1-2-4-8(7)13(15)19/h1-4

InchiKey: UEJJHQNACJXSKW-UHFFFAOYSA-N

Formula: C13H10N2O4

SMILES: O=C1CCC(N2C(=O)c3ccccc3C2=O)C(=O)N1

Mol. weight [g/mol]: 258.23

CAS: 50-35-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Aqueous Solubility Prediction Method
log10ws	-2.68		Estimated Solubility Method
logp	0.088		Crippen Method
mcvol	174.790	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	36.02	kJ/mol	548.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50351&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume