Phenytoin

Other names:

10-oxo-10,11-dihydro-5H-dibenzo[b,f]azepine-5-carboxamide
2,4-Imidazolidinedione, 5,5-diphenyl-
5,5-Diphenyl-1H-imidazolidine-2,4-dione
5,5-Diphenyl-2,4-Imidazolidinedione
5,5-Diphenyl-2,4-imidazolidinedione (phenytoin)
5,5-Diphenylhydantoin
5,5-Diphenylimidazolidin-2,4-dione
5,5-Dwufenylohydantoina
5,5-diphenylimidazolidine-2,4-dione
Aleviatin
Auranile
Causoin
Citrulliamon
Comitoina
Convul
DPH
Danten
Dantinal
Dantoinal
Dantoinal klinos
Dantoine
Denyl
Di-Hydan
Di-Lan
Di-Phetine
Didan TDC 250
Difenilhidantoina
Difenin
Difetoin
Difhydan
Dihycon
Dihydantoin
Dilabid
Dilantin
Dilantin acid
Dilantine
Dillantin
Dintoin
Dintoina
Diphantoin

Diphedal
Diphedan
Diphenat
Diphenin
Diphenine
Diphentoin
Diphentyn
Diphenylan
Diphenylhydantoin
Diphenylhydantoine
Diphenylhydatanoin
Ditoinate
Ekko
Ekko capsules
Elepsindon
Enkelfel
Epamin
Epanutin
Epasmir "5"
Epdantoine simple
Epelin
Epifenyl
Epihydan
Epilan-D
Epilantin
Epinat
Epised
Eptal
Eptoin
Fenidantoin "s"
Fenitoina
Fentoin
Fenylepsin
Fenytoine
Gerot-epilan-D
Hidan
Hidantal
Hidantilo
Hidantina
Hidantina senosian
Hidantina vitoria
Hidantomin
Hindatal

Hydantal
Hydantin
Hydantoin, 5,5-diphenyl-
Hydantoinal
Ictalis simple
Idantoil
Idantoin
Kessodanten
Labopal
Lehydan
Lepitoin
Lepsin
Minetoin
NCI-C55765
Neos-Hidantoina
Neosidantoina
Novantoina
Om hidantoina simple
Om-Hydantoine
Oxacarbazepine
Oxcarbazepine
Oxylan
Phanantin
Phanatine
Phenatine
Phenatoine
Phenitoin
Phentoin
Phenytoine
Ritmenal
Saceril
Sanepil
Silantin
Sodantoin
Sodanton
Solantin
Solantoin
Solantyl
Sylantoic
TOIN
Thilophenyl
Toin unicelles
Zentronal

	Zentropil
Inchi:	InChI=1S/C15H12N2O2/c18-13-15(17-14(19)16-13,11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1
InchiKey:	CXOFVDLJLONNDW-UHFFFAOYSA-N
Formula:	C15H12N2O2
SMILES:	O=C1NC(=O)C(c2ccccc2)(c2ccccc2)N1
Mol. weight [g/mol]:	252.27
CAS:	57-41-0

Physical Properties

Property code	Value	Unit	Source
gf	261.54	kJ/mol	Joback Method
hf	-3.93	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-4.10		Estimated Solubility Method
log10ws	-3.93		Aqueous Solubility Prediction Method
logp	1.770		Crippen Method
mcvol	186.930	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2369.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2365.00		NIST Webbook
rinpol	2369.00		NIST Webbook
rinpol	2340.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2385.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	844.22	K	Joback Method
tc	1147.60	K	Joback Method

tf	567.07	K	Aqueous Solubility Prediction Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.04	J/mol×K	894.78	Joback Method
cpg	590.01	J/mol×K	945.35	Joback Method
cpg	606.19	J/mol×K	995.91	Joback Method
cpg	621.77	J/mol×K	1046.47	Joback Method
cpg	636.96	J/mol×K	1097.04	Joback Method
cpg	555.05	J/mol×K	844.22	Joback Method
cpg	651.96	J/mol×K	1147.60	Joback Method
hfust	40.10	kJ/mol	568.80	NIST Webbook
hfust	47.08	kJ/mol	570.80	NIST Webbook
hfust	36.29	kJ/mol	574.00	NIST Webbook
hfust	36.29	kJ/mol	574.00	NIST Webbook
hvapt	140.00	kJ/mol	520.00	Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Experimental investigation and modeling of the solubility of oxcarbazepine (an anticonvulsant drug) in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2019.04.013
Evaluation of sublimation enthalpy by thermogravimetry: Analysis of the diffusion effects in the case of methyl and phenyl substituted hydantoins:	https://www.doi.org/10.1016/j.tca.2017.06.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume