Phenobarbital

Other names:

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-phenyl-
5-Ethyl-5-phenyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Ethyl-5-phenylbarbituric acid
5-Phenyl-5-ethylbarbituric acid
5-ethyl-5-phenyl-2,4,6-(1H,3H,5H)pyrmidinetrione
Adonal
Aephenal
Agrypnal
Amylofene
Aphenylbarbit
Aphenyletten
Barbenyl
Barbilehae (barbilettae)
Barbinal
Barbiphen
Barbiphenyl
Barbipil
Barbita
Barbituric acid, 5-ethyl-5-phenyl-
Barbivis
Barbonal
Barbophen
Bardorm
Bartol
Bialminal
Blu-phen
Cabronal
Calmetten
Calminal
Cardenal
Chinoin
Codibarbita
Coronaletta
Cratecil
Damoral
Dezibarbitur
Dormina
Dormiral
Dormital
Doscalun

Duneryl
Ensobarb
Ensodorm
Epanal
Epidorm
Epilol
Episedal
Epsylone
Eskabarb
Etilfen
Euneryl
Fenbital
Fenemal
Fenemal recip
Fenobarbital
Fenosed
Fenylettae
Gardenal
Gardepanyl
Glysoletten
Haplopan
Haplos
Helional
Hennoletten
Henotal
Hypnaletten
Hypnette
Hypno-Tablinetten
Hypnogen
Hypnolone
Hypnoltol
Hysteps
Lefebar
Leonal
Lephebar
Lepinal
Lepinaletten
Linasen
Liquital
Lixophen
Lubergal
Lubrokal
Lumen

Lumesettes
Lumesyn
Luminal
Lumofridetten
Luphenil
Luramin
Mephobarbital M (nor)
Methylphenobarbital, M(nor-)
Molinal
Neurobarb
Nirvonal
Noptil
Nova-Pheno
Nunol
Parkotal
Pharmetten
Phen-Bar
Phenaemal
Phenemal
Phenemalum
Phenobal
Phenobar
Phenobarbitol
Phenobarbitone
Phenobarbituric acid
Phenobarbyl
Phenoluric
Phenolurio
Phenomet
Phenonyl
Phenoturic
Phenylethylbarbiturate
Phenylethylbarbituric acid
Phenylethylmalonylurea
Phenyletten
Phenyral
Phob
Polcominal
Primidone, M (phenobarbital)
Promptonal
SK-Phenobarbital
Seda-Tablinen
Sedabar

Sedicat
Sedizorin
Sedlyn
Sedofen
Sedonal
Sedonal (sedative)
Sedonettes
Sedophen
Sevenal
Sinoratox
Solfoton
Solfoton talpheno
Solu-Barb
Sombutol
Somnolens
Somnoletten
Somnosan
Somonal
Spasepilin
Starifen
Starilettae
Stental
Stental Extentabs
Talpheno
Teolaxin
Teoloxin
Thenobarbital
Theoloxin
Triabarb
Tridezibarbitur
Triphenatol
Versomnal
Zadoletten
Zadonal
component of Antrocol
component of Barbidonna
component of Bronkotabs
component of Chardonna-2
component of Donnatal
component of Donnazyme
component of Hecadrol
component of Hydantal
component of Kinesed

component of Levsin pb drops and tablets
component of Primatene P
component of Quadrinal
component of Slowten
component of Tedral
component of Valpin 50-PB
pyrimidinetrione, 5-ethyl-5-phenyl-2,4,6-(1H,3H,5H)-

Inchi: InChI=1S/C12H12N2O3/c1-2-12(8-6-4-3-5-7-8)9(15)13-11(17)14-10(12)16/h3-7H,2H2,1H

InchiKey: DDBREPKUVSBGFI-UHFFFAOYSA-N

Formula: C12H12N2O3

SMILES: CCC1(c2ccccc2)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 232.24

CAS: 50-06-6

Physical Properties

Property code	Value	Unit	Source
gf	-10.82	kJ/mol	Joback Method
hf	-322.40	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	70.12	kJ/mol	Joback Method
log10ws	-2.35		Aqueous Solubility Prediction Method
log10ws	-2.32		Estimated Solubility Method
logp	0.700		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1922.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1984.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1934.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1955.00		NIST Webbook

rinpol	1955.00	NIST Webbook
rinpol	1960.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1939.00	NIST Webbook
rinpol	1938.00	NIST Webbook
rinpol	1990.00	NIST Webbook
rinpol	1975.00	NIST Webbook
rinpol	1970.00	NIST Webbook
rinpol	1944.00	NIST Webbook
rinpol	1928.00	NIST Webbook
rinpol	1960.00	NIST Webbook
rinpol	1995.00	NIST Webbook
rinpol	1928.00	NIST Webbook
rinpol	1975.00	NIST Webbook
rinpol	1924.00	NIST Webbook
rinpol	1964.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1955.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1934.00	NIST Webbook
rinpol	1996.00	NIST Webbook
rinpol	1957.00	NIST Webbook
rinpol	1926.00	NIST Webbook
rinpol	1928.00	NIST Webbook
rinpol	1922.00	NIST Webbook
rinpol	1935.00	NIST Webbook
rinpol	1975.00	NIST Webbook
rinpol	1975.00	NIST Webbook
rinpol	1980.00	NIST Webbook
rinpol	1957.00	NIST Webbook
rinpol	1924.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1957.00	NIST Webbook
rinpol	1954.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1964.00	NIST Webbook
rinpol	1990.00	NIST Webbook
rinpol	1965.00	NIST Webbook
rinpol	1939.00	NIST Webbook
rinpol	1984.00	NIST Webbook

rinpol	1934.00		NIST Webbook
rinpol	1921.50		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	820.99	K	Joback Method
tc	1110.83	K	Joback Method
tf	449.00 ± 4.00	K	NIST Webbook
tf	447.98	K	Aqueous Solubility Prediction Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.92	J/mol×K	820.99	Joback Method
cpg	530.54	J/mol×K	869.30	Joback Method
cpg	546.92	J/mol×K	917.60	Joback Method
cpg	562.11	J/mol×K	965.91	Joback Method
cpg	576.14	J/mol×K	1014.22	Joback Method
cpg	589.07	J/mol×K	1062.52	Joback Method
cpg	600.92	J/mol×K	1110.83	Joback Method

Sources

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

Solubility of Lamotrigine, Diazepam, Clonazepam, and Phenobarbital in Propylene Glycol + Water Mixtures at 298.15 K: https://www.doi.org/10.1021/je800931z

Solubility of Clonazepam, Diazepam, Lamotrigine, and Phenobarbital in N-Methyl-2-pyrrolidone + Water Mixtures at 298.2 K: https://www.doi.org/10.1021/je9000153

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50066&Units=SI

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
hvap:	Enthalpy of vaporization at standard conditions
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