Primidone

Other names:

2-Deoxyphenobarbital
2-Desoxyphenobarbital
4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-phenyl-
5-Aethyl-5-phenyl-hexahydropyrimidin-4,6-dion
5-Ethyl-5-phenylhexahydropyrimidine-4,6-dione
5-Ethyldihydro-5-phenyl-4,6(1H,5H)-pyrimidinedione
5-Ethylhexahydro-4,6-dioxo-5-phenylpyrimidine
5-Ethylhexahydro-5-phenylpyrimidine-4,6-dione
5-Phenyl-5-aethylhexahydropyrimidindion-(4,6)
5-Phenyl-5-ethyl-hexahydropyrimidine-4,6-dione
Cyral
Desoxyphenobarbitone
Hexadiona
Hexamidine
Lepimidin
Lepsiral
Liskantin
Majsolin
Medi-Pets
Midone
Milepsin
Misodine
Misolyne
Mizodin
Mizolin
Mylepsin
Mylepsinum
Mysedon
Mysoline
NCI-C56360
NSC 41701
Neurosyn
Prilepsin
Primacione
Primaclone
Primacone
Primakton
Primidon
Primoline
Prysoline

	Pyrimidone "Medi-pets"
	Pyrimidone Medi-pets
	Resimatil
	Roe 101
	Sertan
Inchi:	InChI=1S/C12H14N2O2/c1-2-12(9-6-4-3-5-7-9)10(15)13-8-14-11(12)16/h3-7H,2,8H2,1H3
InchiKey:	DQMZLTXERSFNPB-UHFFFAOYSA-N
Formula:	C12H14N2O2
SMILES:	CCC1(c2ccccc2)C(=O)NCNC1=O
Mol. weight [g/mol]:	218.25
CAS:	125-33-7

Physical Properties

Property code	Value	Unit	Source
gf	111.77	kJ/mol	Joback Method
hf	-184.70	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-2.64		Estimated Solubility Method
log10ws	-2.48		Aqueous Solubility Prediction Method
logp	0.538		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
rinpol	2247.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2243.00		NIST Webbook
rinpol	2202.00		NIST Webbook
rinpol	2324.50		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2225.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2247.00		NIST Webbook
tb	753.17	K	Joback Method
tc	1033.89	K	Joback Method
tf	554.53	K	Aqueous Solubility Prediction Method

vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.22	J/mol×K	753.17	Joback Method
cpg	504.76	J/mol×K	799.96	Joback Method
cpg	522.21	J/mol×K	846.74	Joback Method
cpg	538.66	J/mol×K	893.53	Joback Method
cpg	554.24	J/mol×K	940.32	Joback Method
cpg	569.04	J/mol×K	987.11	Joback Method
cpg	583.18	J/mol×K	1033.89	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125337&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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