HEPTOBARBITAL

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-phenyl-
	5-Methyl-5-phenyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-Methyl-5-phenylbarbituric acid
	5-Methyl-5-phenylbarbityric acid
	5-Phenyl-5-methylbarbituric acid
	5-methyl-5-phenyl-1,3-diazinane-2,4,6-trione
	Barbituric acid, 5-methyl-5-phenyl-
	Eudan
	Mephebarbital
	Methylphenylbarbital
	NSC 80543
	Rutonal
Inchi:	InChI=1S/C11H10N2O3/c1-11(7-5-3-2-4-6-7)8(14)12-10(16)13-9(11)15/h2-6H,1H3,(H2,1
InchiKey:	LSAOZCAKUIANSQ-UHFFFAOYSA-N
Formula:	C11H10N2O3
SMILES:	CC1(c2ccccc2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	218.21

Physical Properties

Property code	Value	Unit	Source
hfus	21.53	kJ/mol	Joback Method
ie	9.03	eV	Cheméo Relay (1.0)
log10ws	-2.46		Aqueous Solubility Prediction Method
logp	0.310		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
rinpol	1860.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tf	497.40	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	457.83	J/mol×K	798.11	Joback Method
cpg	475.06	J/mol×K	847.76	Joback Method
cpg	491.09	J/mol×K	897.42	Joback Method
cpg	505.95	J/mol×K	947.07	Joback Method
cpg	519.67	J/mol×K	996.73	Joback Method
cpg	532.30	J/mol×K	1046.38	Joback Method
cpg	543.87	J/mol×K	1096.03	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76948&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point