

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(4-hydroxyphenyl)-

Other names:

Hydroxyphenobarbitone,p-

Phenobarbital-p-hydroxy

4-Hydroxyphenobarbital

5-ethyl-5-(4'-hydroxyphenyl)barbituric acid monohydrate

Inchi:

InChI=1S/C12H12N2O4/c1-2-12(7-3-5-8(15)6-4-7)9(16)13-11(18)14-10(12)17/h3-6,15H,

InchiKey:

IEPXMJKJNWPXDBP-UHFFFAOYSA-N

Formula:

C12H12N2O4

SMILES:

CCC1(c2ccc(O)cc2)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]:

248.23

CAS:

379-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-165.44	kJ/mol	Joback Method
hf	-499.71	kJ/mol	Joback Method
hfus	29.91	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	0.406		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
tb	901.61	K	Joback Method
tc	1194.26	K	Joback Method
tf	809.14	K	Joback Method
vc	0.592	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.26	J/mol×K	901.61	Joback Method
cpg	578.07	J/mol×K	950.38	Joback Method
cpg	594.28	J/mol×K	999.16	Joback Method

cpg	610.02	J/mol×K	1047.93	Joback Method
cpg	625.42	J/mol×K	1096.71	Joback Method
cpg	640.63	J/mol×K	1145.48	Joback Method
cpg	655.77	J/mol×K	1194.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C379340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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