

5-Ethyl-5-(4-acetoxyphenyl)-hexahydropyrimidin-2(1H)-one

Other names:	Phenobarbital M (OH), acetylated Mephobarbital M (nor-OH), acetylated Phenobarbital, M (HO-), AC Methylphenobarbital, M (nor-HO-), AC Primidone, M (HO-phenobarbital), AC
Inchi:	InChI=1S/C14H14N2O5/c1-3-14(11(18)15-13(20)16-12(14)19)9-4-6-10(7-5-9)21-8(2)17/1
InchiKey:	RQDKDIOGKDBEOA-UHFFFAOYSA-N
Formula:	C14H14N2O5
SMILES:	CCC1(c2ccc(OC(C)=O)cc2)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	290.27

Physical Properties

Property code	Value	Unit	Source
gf	-237.53	kJ/mol	Joback Method
hf	-619.95	kJ/mol	Joback Method
hfus	31.70	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	0.626		Crippen Method
mcvol	205.610	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	948.02	K	Joback Method
tc	1222.82	K	Joback Method
tf	804.64	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	662.94	J/mol×K	948.02	Joback Method
cpg	677.89	J/mol×K	993.82	Joback Method
cpg	691.37	J/mol×K	1039.62	Joback Method
cpg	703.40	J/mol×K	1085.42	Joback Method
cpg	713.96	J/mol×K	1131.22	Joback Method
cpg	723.05	J/mol×K	1177.02	Joback Method
cpg	730.67	J/mol×K	1222.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U281592&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

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