Barbituric acid, 5-allyl-5-phenyl-

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-phenyl-5-(2-propenyl)-
5-Allyl-5-phenyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-phenyl-barbituric acid (alphenal)
5-Allyl-5-phenylbarbital
5-Allyl-5-phenylbarbituric acid
5-Phenyl-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Phenyl-5-allylbarbituric acid
Acido 5-fenil-5-allilbarbiturico
Allofenyl
Allophenylum
Alphasem
Alpheba
Alphenal
Alphenate
Dorlotin
Fenallymal
Lubergal
Luxomnin
Phenallymal
Phenallymalum
Phenyral
Prophenal
Tubergal

Inchi: InChI=1S/C13H12N2O3/c1-2-8-13(9-6-4-3-5-7-9)10(16)14-12(18)15-11(13)17/h2-7H,1,8

InchiKey: WOIGZSBYKGQJGL-UHFFFAOYSA-N

Formula: C13H12N2O3

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

Mol. weight [g/mol]: 244.25

CAS: 115-43-5

Physical Properties

Property code	Value	Unit	Source
gf	85.44	kJ/mol	Joback Method
hf	-217.61	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	71.67	kJ/mol	Joback Method

log10ws	-2.37		Estimated Solubility Method
log10ws	-2.35		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.18		Aqueous Solubility Prediction Method
logp	0.867		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	2106.00		NIST Webbook
rinpol	2089.50		NIST Webbook
rinpol	2106.00		NIST Webbook
tb	840.55	K	Joback Method
tc	1128.85	K	Joback Method
tf	429.90	K	Aqueous Solubility Prediction Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.12	J/mol×K	840.55	Joback Method
cpg	559.48	J/mol×K	888.60	Joback Method
cpg	575.64	J/mol×K	936.65	Joback Method
cpg	590.66	J/mol×K	984.70	Joback Method
cpg	604.60	J/mol×K	1032.75	Joback Method
cpg	617.51	J/mol×K	1080.80	Joback Method
cpg	629.46	J/mol×K	1128.85	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C115435&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

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