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

Other names: 5-Allyl-5-ethylbarbituric acid
5-allyl-5-ethylbarbital
Aethallymal
Barbituric acid, 5-allyl-5-ethyl-

Inchi: InChI=1S/C9H12N2O3/c1-3-5-9(4-2)6(12)10-8(14)11-7(9)13/h3H,1,4-5H2,2H3,(H2,10,11

InchiKey: QPADNTZLUBYNEN-UHFFFAOYSA-N

Formula: C9H12N2O3

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

Mol. weight [g/mol]: 196.20

CAS: 2373-84-4

Physical Properties

Property code	Value	Unit	Source
gf	-60.65	kJ/mol	Joback Method
hf	-371.58	kJ/mol	Joback Method
hfus	21.03	kJ/mol	Joback Method
hvap	60.49	kJ/mol	Joback Method
log10ws	-1.61		Aqueous Solubility Prediction Method
log10ws	-1.61		Estimated Solubility Method
log10ws	-1.61		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.325		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1532.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	722.35	K	Joback Method
tc	986.65	K	Joback Method
tf	635.43	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.24	J/mol×K	722.35	Joback Method
cpg	432.85	J/mol×K	766.40	Joback Method
cpg	448.64	J/mol×K	810.45	Joback Method
cpg	463.61	J/mol×K	854.50	Joback Method
cpg	477.77	J/mol×K	898.55	Joback Method
cpg	491.14	J/mol×K	942.60	Joback Method
cpg	503.71	J/mol×K	986.65	Joback Method

Sources

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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=C2373844&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

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