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

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-butyl-5-(2-propen-1-yl)-
5-Allyl-5-butyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-n-butylbarbituric acid
5-Butyl-5-allylbarbituric acid
5-butyl-5-prop-2-enyl-1,3-diazinane-2,4,6-trione
Allylbutylbarbituric acid
Barbituric acid, 5-allyl-5-butyl-
Barbituric acid, 5-butyl-5-(2-propenyl)
Idobutal
n-Butylallylbarbitone
n-Butylallylbarbituric acid

Inchi: InChI=1S/C11H16N2O3/c1-3-5-7-11(6-4-2)8(14)12-10(16)13-9(11)15/h4H,2-3,5-7H2,1H3

InchiKey: RRWVWLGUQPLOMY-UHFFFAOYSA-N

Formula: C11H16N2O3

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

Mol. weight [g/mol]: 224.26

Physical Properties

Property code	Value	Unit	Source
hfus	26.21	kJ/mol	Joback Method
log10ws	-2.17		Aqueous Solubility Prediction Method
logp	1.105		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tf	402.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.20	J/mol×K	768.11	Joback Method

cpg	541.90	J/mol×K	810.17	Joback Method
cpg	558.67	J/mol×K	852.23	Joback Method
cpg	574.55	J/mol×K	894.29	Joback Method
cpg	589.53	J/mol×K	936.36	Joback Method
cpg	603.64	J/mol×K	978.42	Joback Method
cpg	616.91	J/mol×K	1020.48	Joback Method

Sources

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=C3146665&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

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

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