5-Allyl-5-butylbarbituric acid

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-butyl-5-(2-propen-1-yl)-
	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-butyl-5-(2-propenyl)-
	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
CAS:	3146-66-5

Physical Properties

Property code	Value	Unit	Source
gf	-43.81	kJ/mol	Joback Method
hf	-412.86	kJ/mol	Joback Method
hfus	26.21	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-2.17		Aqueous Solubility Prediction Method
logp	1.105		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	768.11	K	Joback Method
tc	1020.48	K	Joback Method
tf	657.97	K	Joback Method

vc	0.658	m3/kmol	Joback Method

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3146665&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