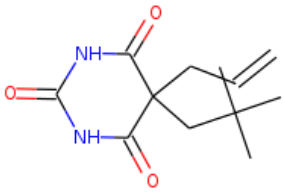
Barbituric acid, 5-allyl-5-neopentyl-

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2,2-dimethylpropyl)-5-(2-propenyl)-; 5-(2,2-Dimethylpropyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione; 5-Allyl-5-(2,2-dimethylpropyl)barbituric acid; 5-Allyl-5-neopentylbarbituric acid; 5-Neopentyl-5-allylbarbituric acid; 5055; Allylneopentylbarbituric acid; Censedal; Nealbarbital; Nealbarbitone; Neallymal; Nepental; Nevental.



InChI: InChI=1S/C12H18N2O3/c1-5-6-12(7-11(2,3)4)8(15)13-10(17)14-9(12)16/h5H,1,6-7H2,2-4H3,(H2,13,14,15,16,17)

InChI Key: YHKPTICJRUESOY-UHFFFAOYSA-N

Formula: C12H18N2O3

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

Molecular Weight: 238.28

CAS: 561-83-1

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-32.55	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-442.25	kJ/mol	Joback Method
$\Delta_{fus} H°$	21.39	kJ/mol	Joback Method
$\Delta_{vap} H°$	65.87	kJ/mol	Joback Method
$logP_{oct/wat}$	1.35		Crippen Method
P_c	2758.46	kPa	Joback Method
T_{boil}	787.76	K	Joback Method
T_c	1048.64	K	Joback Method
T_{fus}	671.66	K	Joback Method
V_c	0.70	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	581.76	J/mol×K	787.76	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H18N2O3/c1-5-6-12(7-11(2,3)4)8(15)13-10(17)14-9(12)16/h5H,1,6-7H2,2-4H3,(H2,13,14,15,16,17)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).