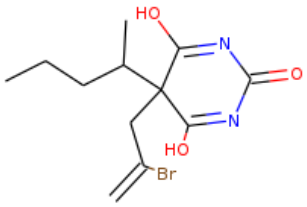
5-(«beta»-Bromoallyl)-5-(1-methylbutyl)barbituric acid



Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(2-bromo-2-propenyl)-5-(1-methylbutyl)-; 5-(2-bromoallyl)-5-(1-methylbutyl)-1H,3H,5H-pyrimidine-2,4,6-trione; Barbituric acid, 5-(2-bromoallyl)-5-(1-methylbutyl)-; R 239; Recton; Sigmodal.

InChI: InChI=1S/C12H17BrN2O3/c1-4-5-7(2)12(6-8(3)13)9(16)14-11(18)15-10(12)17/h7H,3-6H2,1-2H3,(H2,14,15,16,17,18)

InChI Key: ZGVCLZRQOUEZHG-UHFFFAOYSA-N

Formula: C12H17BrN2O3

SMILES: C=C(Br)CC1(C(C)CCC)C(O)=NC(=O)N=C1O

Molecular Weight: 317.18

CAS: 1216-40-6

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	38.28	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-292.36	kJ/mol	Joback Method
$\Delta_{fus} H°$	31.17	kJ/mol	Joback Method
$\Delta_{vap} H°$	98.97	kJ/mol	Joback Method
$logP_{oct/wat}$	3.75		Crippen Method
P_c	3329.68	kPa	Joback Method
T_{boil}	923.89	K	Joback Method
T_c	1150.89	K	Joback Method
T_{fus}	644.86	K	Joback Method
V_c	0.79	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	663.07	J/mol×K	923.89	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17BrN2O3/c1-4-5-7(2)12(6-8(3)13)9(16)14-11(18)15-10(12)17/h7H,3-6H2,1-2H3,(H2,14,15,16,17,18)

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: 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).