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)-
Barbituric acid, 5-(2-bromoallyl)-5-(1-methylbutyl)-
R 239
Recton
Sigmodal
5-(2-bromoallyl)-5-(1-methylbutyl)-1H,3H,5H-pyrimidine-2,4,6-trione

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

InchiKey: ZGVCLZRQOUEZHG-UHFFFAOYSA-N

Formula: C12H17BrN2O3

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

Mol. weight [g/mol]: 317.18

CAS: 1216-40-6

Physical Properties

Property code	Value	Unit	Source
gf	38.28	kJ/mol	Joback Method
hf	-292.36	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	98.97	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.754		Crippen Method
mcvol	206.950	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
tb	923.89	K	Joback Method
tc	1150.89	K	Joback Method
tf	644.86	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.07	J/mol×K	923.89	Joback Method

cpg	676.07	J/mol×K	961.72	Joback Method
cpg	688.58	J/mol×K	999.56	Joback Method
cpg	700.67	J/mol×K	1037.39	Joback Method
cpg	712.43	J/mol×K	1075.22	Joback Method
cpg	723.94	J/mol×K	1113.05	Joback Method
cpg	735.25	J/mol×K	1150.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1216406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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