2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-hydroxy-1-methylbutyl)-

Other names: Barbituric acid, 5-ethyl-5-(3-hydroxy-1-methylbutyl)-
Hydroxypentobarbital
Hydroxypentobarbitone
3'-Hydroxypentobarbitone
3'-Hydroxypentobarbital

Inchi: InChI=1S/C11H18N2O4/c1-4-11(6(2)5-7(3)14)8(15)12-10(17)13-9(11)16/h6-7,14H,4-5H2

InchiKey: XYOPMDJVSWQZTM-UHFFFAOYSA-N

Formula: C11H18N2O4

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

Mol. weight [g/mol]: 242.27

CAS: 4241-40-1

Physical Properties

Property code	Value	Unit	Source
gf	-273.35	kJ/mol	Joback Method
hf	-701.08	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	81.52	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	0.156		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
tb	862.73	K	Joback Method
tc	1099.90	K	Joback Method
tf	690.55	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.57	J/mol×K	862.73	Joback Method
cpg	624.14	J/mol×K	902.26	Joback Method

cpg	638.81	J/mol×K	941.79	Joback Method
cpg	652.60	J/mol×K	981.32	Joback Method
cpg	665.51	J/mol×K	1020.84	Joback Method
cpg	677.56	J/mol×K	1060.37	Joback Method
cpg	688.76	J/mol×K	1099.90	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4241401&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