Barbituric acid, 5-ethyl-5-(1-methyl-2-butenyl)-

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methyl-2-butenyl)-
5-Ethyl-5-(1-methyl-2-butenyl)barbituric acid
5-Ethyl-5-(1-methyl-3-butenyl)-hexahydropyrimidin-2,4,6-trione
5-Ethyl-5-(1-methyl-2-butenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
Pentobarbital M (OH, -H2O)

Inchi: InChI=1S/C11H16N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h4,6-7H,5H2,1-3H

InchiKey: PUAFBJFWUGOCOU-GQCTYLIASA-N

Formula: C11H16N2O3

SMILES: CC=CC(C)C1(CC)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 224.26

CAS: 17013-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-53.87	kJ/mol	Joback Method
hf	-426.35	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	0.961		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	775.15	K	Joback Method
tc	1037.31	K	Joback Method
tf	639.65	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.19	J/mol×K	775.15	Joback Method

cpg	543.39	J/mol×K	818.84	Joback Method
cpg	560.64	J/mol×K	862.54	Joback Method
cpg	576.96	J/mol×K	906.23	Joback Method
cpg	592.39	J/mol×K	949.92	Joback Method
cpg	606.96	J/mol×K	993.62	Joback Method
cpg	620.71	J/mol×K	1037.31	Joback Method

Sources

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=C17013353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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