Vinbarbital

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methyl-1-butenyl)-
5-Ethyl-5-(1-methyl-1-butenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Ethyl-5-(1-methyl-1-butenyl)barbiturate
5-Ethyl-5-(1-methyl-1-butenyl)barbituric acid
Barbituric acid, 5-ethyl-5-(1-methyl-1-butenyl)-
Butenemal
Delvinal
Devinal
NSC 117442
Suppoptanox
Vinbarbitone

Inchi: InChI=1S/C11H16N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h6H,4-5H2,1-3H3,(

InchiKey: RAFOHKSPUDGZPR-VOTSOKGWSA-N

Formula: C11H16N2O3

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

Mol. weight [g/mol]: 224.26

CAS: 125-42-8

Physical Properties

Property code	Value	Unit	Source
gf	-59.98	kJ/mol	Joback Method
hf	-430.86	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	65.65	kJ/mol	Joback Method
log10ws	-2.31		Aqueous Solubility Prediction Method
logp	1.105		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1755.00		NIST Webbook
tb	775.47	K	Joback Method

tc	1036.79	K	Joback Method
tf	436.00 ± 4.00	K	NIST Webbook
tf	439.00 ± 1.00	K	NIST Webbook
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.28	J/mol×K	775.47	Joback Method
cpg	542.41	J/mol×K	819.02	Joback Method
cpg	559.62	J/mol×K	862.58	Joback Method
cpg	575.93	J/mol×K	906.13	Joback Method
cpg	591.38	J/mol×K	949.68	Joback Method
cpg	606.01	J/mol×K	993.24	Joback Method
cpg	619.86	J/mol×K	1036.79	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C125428&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