Vinylbital

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethenyl-5-(1-methylbutyl)-
	5-(1-Methylbutyl)-5-vinyl-2,4,6(1H,3H,5H)-pyrimidinetrione
	5-(1-Methylbutyl)-5-vinylbarbituric acid
	5-ethenyl-5-pentan-2-yl-1,3-diazinane-2,4,6-trione
	Butylvinal
	Butyvinal
	Bykonox
	JD-96
	Optanox
	Speda
	Vinylbitalum
	Vinylbitone
	Vinymal
Inchi:	InChI=1S/C11H16N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h5,7H,2,4,6H2,1,3H
InchiKey:	KGKJZEKQJQQOTD-UHFFFAOYSA-N
Formula:	C11H16N2O3
SMILES:	C=CC1(C(C)CCC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	224.26
CAS:	2430-49-1

Physical Properties

Property code	Value	Unit	Source
gf	-46.25	kJ/mol	Joback Method
hf	-418.14	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-2.36		Aqueous Solubility Prediction Method
logp	0.961		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1712.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	767.67	K	Joback Method
tc	1025.00	K	Joback Method

tf	363.48	K	Aqueous Solubility Prediction Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.76	J/mol×K	767.67	Joback Method
cpg	542.80	J/mol×K	810.56	Joback Method
cpg	559.87	J/mol×K	853.45	Joback Method
cpg	575.99	J/mol×K	896.34	Joback Method
cpg	591.16	J/mol×K	939.22	Joback Method
cpg	605.41	J/mol×K	982.11	Joback Method
cpg	618.77	J/mol×K	1025.00	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2430491&Units=SI
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

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