5-Ethenyl-5-(1-methyl-3-butenyl)-hexahydropyrim

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethenyl-5-(1-methyl-3-butenyl)-
Vinylbital M (OH, -H2O)
Inchi: InChI=1S/C11H14N2O3/c1-4-6-7(3)11(5-2)8(14)12-10(16)13-9(11)15/h4-5,7H,1-2,6H2,3
InchiKey: DMEKNBFGYSDJIZ-UHFFFAOYSA-N
Formula: C11H14N2O3
SMILES: C=CCC(C)C1(C=C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 222.24
CAS: 131147-55-2

Physical Properties

Property code	Value	Unit	Source
gf	41.59	kJ/mol	Joback Method
hf	-292.71	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	0.737		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	764.35	K	Joback Method
tc	1026.96	K	Joback Method
tf	641.21	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.42	J/mol×K	764.35	Joback Method
cpg	516.86	J/mol×K	808.12	Joback Method
cpg	533.36	J/mol×K	851.89	Joback Method
cpg	548.95	J/mol×K	895.66	Joback Method
cpg	563.65	J/mol×K	939.42	Joback Method

cpg	577.49	J/mol×K	983.19	Joback Method
cpg	590.50	J/mol×K	1026.96	Joback Method

Sources

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=C131147552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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