5,5-DIHYDROXY-2,4,6(1H,3H,5H)-PYRIMIDINETRIO

Other names:	Barbituric acid, 5,5-dihydroxy-
	Mesoxalylcarbamide monohydrate
	Mesoxalylurea monohydrate
	2,4,5,6(1H,3H)-Pyrimidinetetrone hydrate
	2,4,5,6(1H,3H)-Pyrimidinetetrone, monohydrate
	5,5-dihydroxyperhydropyrimidinetrione
	Alloxan
Inchi:	InChI=1S/C4H4N2O5/c7-1-4(10,11)2(8)6-3(9)5-1/h10-11H,(H2,5,6,7,8,9)
InchiKey:	ZIIHZVKHFWOENY-UHFFFAOYSA-N
Formula:	C4H4N2O5
SMILES:	O=C1NC(=O)C(O)(O)C(=O)N1
Mol. weight [g/mol]:	160.09

Physical Properties

Property code	Value	Unit	Source
chs	-1144.70 ± 0.67	kJ/mol	NIST Webbook
hfs	-1004.20	kJ/mol	NIST Webbook
hfus	17.54	kJ/mol	Joback Method
ie	10.15	eV	Cheméo Relay (1.0)
log10ws	-0.79		Cheméo Relay (1.0)
logp	-2.967		Crippen Method
mcvol	92.770	ml/mol	McGowan Method
tf	470.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.94	J/mol×K	795.63	Joback Method
cpg	282.01	J/mol×K	835.49	Joback Method
cpg	290.70	J/mol×K	875.35	Joback Method
cpg	298.99	J/mol×K	915.20	Joback Method
cpg	306.88	J/mol×K	955.06	Joback Method
cpg	314.35	J/mol×K	994.92	Joback Method
cpg	321.38	J/mol×K	1034.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3237501&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point