2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-dihydroxy-

Other names: 2,4,5,6(1H,3H)-Pyrimidinetetrone hydrate
2,4,5,6(1H,3H)-Pyrimidinetetrone, monohydrate
5,5-dihydroxyperhydropyrimidinetrione
Alloxan
Barbituric acid, 5,5-dihydroxy-
Mesoxalylcarbamide monohydrate
Mesoxalylurea monohydrate

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: $C_4H_4N_2O_5$

SMILES: O=C1NC(=O)C(O)(O)C(=O)N1

Mol. weight [g/mol]: 160.09

CAS: 3237-50-1

Physical Properties

Property code	Value	Unit	Source
chs	-1144.70 ± 0.67	kJ/mol	NIST Webbook
gf	-464.23	kJ/mol	Joback Method
hf	-698.27	kJ/mol	Joback Method
hfs	-1004.20	kJ/mol	NIST Webbook
hfus	17.54	kJ/mol	Joback Method
hvap	83.39	kJ/mol	Joback Method
log10ws	-1.25		Estimated Solubility Method
log10ws	-1.25		Aqueous Solubility Prediction Method
logp	-2.967		Crippen Method
mcvol	92.770	ml/mol	McGowan Method
pc	9744.98	kPa	Joback Method
tb	795.63	K	Joback Method
tc	1034.78	K	Joback Method
tf	702.48	K	Joback Method
vc	0.324	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3237501&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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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