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: C4H4N2O5

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		Aqueous Solubility Prediction Method
log10ws	-1.25		Estimated Solubility 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

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
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

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