2,4,5,6(1H,3H)-PYRIMIDINETETRONE

Other names:	2,4,5,6(1H,3H)-Pyrimidinetetrone
	Alloxan 7169
	Alloxane
	Barbituric acid, 5-oxo-
	Mesoxalylcarbamide
	Mesoxalylurea
	Urea, mesoxalyl-
	2,4,5,6-Pyrimidintetrone
	2,4,5,6-Tetraoxohexahydropyrimidine
	2,4,5,6-Pyrimidinetetrone
	Pyrimidinetetrone
	NSC 7169
Inchi:	InChI=1S/C4H2N2O4/c7-1-2(8)5-4(10)6-3(1)9/h(H2,5,6,8,9,10)
InchiKey:	HIMXGTXNXJYFGB-UHFFFAOYSA-N
Formula:	C4H2N2O4
SMILES:	O=C1NC(=O)C(=O)C(=O)N1
Mol. weight [g/mol]:	142.07

Physical Properties

Property code	Value	Unit	Source
hfus	14.10	kJ/mol	Joback Method
ie	10.33	eV	Cheméo Relay (1.0)
log10ws	-1.14		Cheméo Relay (1.0)
logp	-2.079		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
ss	153.00	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.39	J/mol×K	683.52	Joback Method
cpg	221.70	J/mol×K	732.52	Joback Method
cpg	233.01	J/mol×K	781.53	Joback Method
cpg	243.00	J/mol×K	830.53	Joback Method

cpg	251.37	J/mol×K	879.53	Joback Method
cpg	257.81	J/mol×K	928.54	Joback Method
cpg	261.99	J/mol×K	977.54	Joback Method
cps	153.01	J/mol×K	297.20	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50715&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
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
ss: Solid phase molar entropy at standard conditions