(S)-2,6-Dioxohexahydro-4-pyrimidinecarboxylic acid

Other names: 2,6-Dioxohexahydro-4-pyrimidinecarboxylic acid- (L)-
Orotic acid, dihydro-, L-
L-5,6-Dihydroorotic acid

Inchi: InChI=1S/C5H6N2O4/c8-3-1-2(4(9)10)6-5(11)7-3/h2H,1H2,(H,9,10)(H2,6,7,8,11)/t2-/m1/s

InchiKey: UFIVEPVSAGBUSI-UWTATZPHSA-N

Formula: C5H6N2O4

SMILES: O=C(O)C1CC(O)=NC(O)=N1

Mol. weight [g/mol]: 158.11

CAS: 5988-19-2

Physical Properties

Property code	Value	Unit	Source
gf	-249.49	kJ/mol	Joback Method
hf	-426.92	kJ/mol	Joback Method
hfus	26.35	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Joback Method
log10ws	0.52		Crippen Method
logp	-0.286		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	8116.22	kPa	Joback Method
tb	779.44	K	Joback Method
tc	982.94	K	Joback Method
tf	555.52	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.13	J/mol×K	779.44	Joback Method
cpg	323.01	J/mol×K	813.36	Joback Method
cpg	329.19	J/mol×K	847.27	Joback Method
cpg	334.67	J/mol×K	881.19	Joback Method
cpg	339.42	J/mol×K	915.11	Joback Method
cpg	343.43	J/mol×K	949.02	Joback Method

cpg	346.66	J/mol×K	982.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5988192&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume