(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-/m0/s

InchiKey: UFIVEPVSAGBUSI-UWTATZPHSA-N

Formula: C5H6N2O4

SMILES: O=C1C[C@@H](C(=O)O)NC(=O)N1

Mol. weight [g/mol]: 158.11

Physical Properties

Property code	Value	Unit	Source
hfus	24.43	kJ/mol	Joback Method
logp	-1.331		Crippen Method
mcvol	100.990	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.36	J/mol×K	712.14	Joback Method
cpg	287.90	J/mol×K	752.47	Joback Method
cpg	297.60	J/mol×K	792.81	Joback Method
cpg	306.37	J/mol×K	833.14	Joback Method
cpg	314.11	J/mol×K	873.47	Joback Method
cpg	320.74	J/mol×K	913.81	Joback Method
cpg	326.17	J/mol×K	954.14	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=C5988192&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume