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

Other names: 5-Hydroxy-2,4,6(1h,3h,5h)-pyrimidinetrione
5-hydroxybarbituric acid
Inchi: InChI=1S/C4H4N2O4/c7-1-2(8)5-4(10)6-3(1)9/h1,7H,(H2,5,6,8,9,10)
InchiKey: BVEWMNTVZPFPQI-UHFFFAOYSA-N
Formula: C4H4N2O4
SMILES: O=C1NC(=O)C(O)C(=O)N1
Mol. weight [g/mol]: 144.09
CAS: 444-15-5

Physical Properties

Property code	Value	Unit	Source
gf	-321.92	kJ/mol	Joback Method
hf	-561.28	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	0.55		Crippen Method
logp	-2.287		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	7561.44	kPa	Joback Method
tb	703.21	K	Joback Method
tc	955.99	K	Joback Method
tf	617.76	K	Joback Method
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.46	J/mol×K	703.21	Joback Method
cpg	248.11	J/mol×K	745.34	Joback Method
cpg	257.92	J/mol×K	787.47	Joback Method
cpg	266.76	J/mol×K	829.60	Joback Method
cpg	274.46	J/mol×K	871.73	Joback Method
cpg	280.86	J/mol×K	913.86	Joback Method
cpg	285.82	J/mol×K	955.99	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C444155&Units=SI
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
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