Barbituric acid

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione
	Malonylurea
	Pyrimidinetrione
	Urea, N,N'-(1,3-dioxo-1,3-propanediyl)-
	2,4,6-Pyrimidinetriol
	2,4,6-Trihydroxypyrimidine
	2,4,6-Trioxohexahydropyrimidine
	6-Hydroxyuracil
	2,4,6-Pyrimidinetrione(1H,3H,5H)
Inchi:	InChI=1S/C4H4N2O3/c7-2-1-3(8)6-4(9)5-2/h1H2,(H2,5,6,7,8,9)
InchiKey:	HNYOPLTXPVRDBG-UHFFFAOYSA-N
Formula:	C4H4N2O3
SMILES:	O=C1CC(=O)NC(=O)N1
Mol. weight [g/mol]:	128.09
CAS:	67-52-7

Physical Properties

Property code	Value	Unit	Source
chs	-1511.10 ± 2.80	kJ/mol	NIST Webbook
chs	-1501.60	kJ/mol	NIST Webbook
gf	-177.39	kJ/mol	Joback Method
hf	-509.70	kJ/mol	NIST Webbook
hfs	-634.70 ± 2.90	kJ/mol	NIST Webbook
hfus	14.59	kJ/mol	Joback Method
hvap	51.49	kJ/mol	Joback Method
ie	10.20	eV	NIST Webbook
log10ws	-0.07		Crippen Method
logp	-1.257		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	6841.44	kPa	Joback Method
ss	157.60	J/mol×K	NIST Webbook
ss	157.30	J/mol×K	NIST Webbook
tb	615.70	K	Joback Method
tc	897.17	K	Joback Method
tf	561.18	K	Joback Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.70	J/mol×K	897.17	Joback Method
cpg	204.75	J/mol×K	662.61	Joback Method
cpg	216.54	J/mol×K	709.52	Joback Method
cpg	227.53	J/mol×K	756.44	Joback Method
cpg	237.53	J/mol×K	803.35	Joback Method
cpg	246.32	J/mol×K	850.26	Joback Method
cpg	192.37	J/mol×K	615.70	Joback Method
cps	141.10	J/mol×K	298.15	NIST Webbook
cps	141.10	J/mol×K	298.15	NIST Webbook
hfust	20.87	kJ/mol	526.40	NIST Webbook
hsubt	113.00 ± 4.00	kJ/mol	442.50	NIST Webbook
hsubt	111.30 ± 0.30	kJ/mol	366.00	NIST Webbook
hsubt	123.30 ± 1.70	kJ/mol	441.50	NIST Webbook

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=C67527&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase 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

hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume