Barbituric acid, 2-thio-

Other names:	4,6(1H,5H)-Pyrimidinedione, dihydro-2-thioxo-
	Bathyran
	Thiobarbituric acid
	2-Mercapto-4,6-dihydroxypyrimidine
	2-Thio-4,6-dioxypyrimidine
	2-Thiobarbituric acid
	4,6(1H,5H)-Pyrimidinedione, 2-mercapto-
	4,6-Dihydroxy-2-thiopyrimidine
	4,6-Dihydroxy-2-mercaptopyrimidine
	USAF EK-660
	Austranal
	2-Mercaptobarbituric acid
	NSC 4733
	1,2,3,4,5,6-Hexahydro-4,6-dioxopyrimidine-2-thione
Inchi:	InChI=1S/C4H4N2O2S/c7-2-1-3(8)6-4(9)5-2/h1H2,(H2,5,6,7,8,9)
InchiKey:	RVBUGGBMJDPOST-UHFFFAOYSA-N
Formula:	C4H4N2O2S
SMILES:	O=C1CC(=O)NC(=S)N1
Mol. weight [g/mol]:	144.15
CAS:	504-17-6

Physical Properties

Property code	Value	Unit	Source
gf	36.05	kJ/mol	Joback Method
hf	-135.91	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	-1.093		Crippen Method
mcvol	91.510	ml/mol	McGowan Method
pc	7181.84	kPa	Joback Method
tb	620.52	K	Joback Method
tc	906.30	K	Joback Method
tf	556.63	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.12	J/mol×K	858.67	Joback Method
cpg	196.08	J/mol×K	620.52	Joback Method
cpg	206.51	J/mol×K	668.15	Joback Method
cpg	216.34	J/mol×K	715.78	Joback Method
cpg	225.45	J/mol×K	763.41	Joback Method
cpg	233.74	J/mol×K	811.04	Joback Method
cpg	247.47	J/mol×K	906.30	Joback Method
hsubt	110.00 ± 4.00	kJ/mol	430.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C504176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsubt:	Enthalpy of sublimation at a given temperature
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