

Isopropylbarbituric acid

Other names:	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)- 5-(1-methylethyl)-2,4,6(1H,3H,5H)-pyrimidinetrione 5-isopropylbarbituric acid 5-isopropylpyrimidine-2,4,6(1H,3H,5H)-trione
Inchi:	InChI=1S/C7H10N2O3/c1-3(2)4-5(10)8-7(12)9-6(4)11/h3-4H,1-2H3,(H2,8,9,10,11,12)
InchiKey:	GFPIGNBQTXNNAG-UHFFFAOYSA-N
Formula:	C7H10N2O3
SMILES:	CC(C)C1C(=O)NC(=O)NC1=O
Mol. weight [g/mol]:	170.17
CAS:	7391-69-7

Physical Properties

Property code	Value	Unit	Source
gf	-162.28	kJ/mol	Joback Method
hf	-476.25	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	-0.375		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	679.23	K	Joback Method
tc	946.14	K	Joback Method
tf	575.75	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.18	J/mol×K	901.65	Joback Method
cpg	341.13	J/mol×K	679.23	Joback Method
cpg	357.38	J/mol×K	723.71	Joback Method
cpg	372.48	J/mol×K	768.20	Joback Method
cpg	386.26	J/mol×K	812.68	Joback Method

cpg	398.55	J/mol×K	857.17	Joback Method
cpg	417.97	J/mol×K	946.14	Joback Method
hvapt	125.00	kJ/mol	298.15	5-Isopropylbarbituric and 2-thiobarbituric acids: An experimental and computational study

Sources

5-Isopropylbarbituric and 2-thiobarbituric acids: An experimental and computational study:	https://www.doi.org/10.1016/j.tca.2015.12.007
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=C7391697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvapt:	Enthalpy of vaporization at a given temperature
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

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