5-Methylbarbituric acid

Inchi: InChI=1S/C5H6N2O3/c1-2-3(8)6-5(10)7-4(2)9/h2H,1H3,(H2,6,7,8,9,10)
InchiKey: GOMAEJQBTWAPAN-UHFFFAOYSA-N
Formula: C5H6N2O3
SMILES: CC1C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 142.11

Physical Properties

Property code	Value	Unit	Source
gf	-176.68	kJ/mol	Joback Method
hf	-429.69	kJ/mol	Joback Method
hfus	18.25	kJ/mol	Joback Method
hvap	53.41	kJ/mol	Joback Method
log10ws	-1.13		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-1.011		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
tb	633.91	K	Joback Method
tc	908.47	K	Joback Method
tf	568.21	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.95	J/mol×K	633.91	Joback Method
cpg	256.06	J/mol×K	679.67	Joback Method
cpg	269.41	J/mol×K	725.43	Joback Method
cpg	281.79	J/mol×K	771.19	Joback Method
cpg	293.00	J/mol×K	816.95	Joback Method
cpg	302.84	J/mol×K	862.71	Joback Method
cpg	311.12	J/mol×K	908.47	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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