Uramil

Other names: 5-aminobarbituric acid
Inchi: InChI=1S/C4H5N3O3/c5-1-2(8)6-4(10)7-3(1)9/h1H,5H2,(H2,6,7,8,9,10)
InchiKey: PSQZLWHRJMYZHD-UHFFFAOYSA-N
Formula: C4H5N3O3
SMILES: NC1C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 143.10
CAS: 118-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-118.65	kJ/mol	Joback Method
hf	-375.26	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	61.83	kJ/mol	Joback Method
log10ws	0.38		Crippen Method
logp	-2.320		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	7121.37	kPa	Joback Method
tb	683.56	K	Joback Method
tc	969.98	K	Joback Method
tf	640.20	K	Joback Method
vc	0.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.84	J/mol×K	683.56	Joback Method
cpg	259.76	J/mol×K	731.30	Joback Method
cpg	271.64	J/mol×K	779.03	Joback Method
cpg	282.26	J/mol×K	826.77	Joback Method
cpg	291.38	J/mol×K	874.51	Joback Method
cpg	298.78	J/mol×K	922.24	Joback Method
cpg	304.24	J/mol×K	969.98	Joback Method

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=C118785&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
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