

4H-Pyran-4-one, 2,6-dimethyl-

Other names:	2,6-Dimethyl-4H-pyran-4-one 2,6-Dimethyl-g-pyrone 2,6-Dimethyl-pyran-4-one 2,6-Dimethyl-«gamma»-pyrone 2,6-dimethyl-.gamma.-pyrone 2,6-dimethyl-4-pyranone 2,6-dimethyl-4-pyrone «gamma»-2,6-Dimethylpyrone
Inchi:	InChI=1S/C7H8O2/c1-5-3-7(8)4-6(2)9-5/h3-4H,1-2H3
InchiKey:	VSYFZULSKMFUJJ-UHFFFAOYSA-N
Formula:	C7H8O2
SMILES:	<chem>Cc1cc(=O)cc(C)o1</chem>
Mol. weight [g/mol]:	124.14
CAS:	1004-36-0

Physical Properties

Property code	Value	Unit	Source
affp	941.50	kJ/mol	NIST Webbook
basg	907.30	kJ/mol	NIST Webbook
ie	9.03	eV	NIST Webbook
log10ws	-5.58		Crippen Method
logp	1.257		Crippen Method
mcvol	97.470	ml/mol	McGowan Method
tb	522.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	86.80	kJ/mol	298.15	When theory and experiment hold hands: The thermochemistry of gamma-pyrone derivatives

Sources

When theory and experiment hold hands: The thermochemistry of gas-phase pyrene derivatives:

NIST Webbook:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.jct.2011.02.021>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1004360&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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