

2H-Pyran-2-one, 3,6-dihydro

Inchi:	InChI=1S/C5H6O2/c6-5-3-1-2-4-7-5/h1-2H,3-4H2
InchiKey:	VREFDQNWPNZEX-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	O=C1CC=CCO1
Mol. weight [g/mol]:	98.10

Physical Properties

Property code	Value	Unit	Source
gf	-155.37	kJ/mol	Joback Method
hf	-283.79	kJ/mol	Joback Method
hfus	8.18	kJ/mol	Joback Method
hvap	36.51	kJ/mol	Joback Method
log10ws	-0.53		Crippen Method
logp	0.489		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	5116.65	kPa	Joback Method
rinpol	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
tb	431.95	K	Joback Method
tc	664.11	K	Joback Method
tf	253.28	K	Joback Method
vc	0.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.36	J/molxK	431.95	Joback Method
cpg	148.11	J/molxK	470.64	Joback Method
cpg	158.40	J/molxK	509.34	Joback Method
cpg	168.20	J/molxK	548.03	Joback Method
cpg	177.50	J/molxK	586.72	Joback Method
cpg	186.29	J/molxK	625.41	Joback Method
cpg	194.57	J/molxK	664.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R89374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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