

2H-Pyran-2-one, 5,6-dihydro-

Other names:	5,6-Dihydro-2H-pyran-2-one 2-Pentenoic acid, 5-hydroxy-, «delta»-lactone 5,6-Dihydro-2-pyranone
Inchi:	InChI=1S/C5H6O2/c6-5-3-1-2-4-7-5/h1,3H,2,4H2
InchiKey:	QBDAFARLDLCWAT-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	O=C1C=CCCO1
Mol. weight [g/mol]:	98.10
CAS:	3393-45-1

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
ripol	1838.00		NIST Webbook
ripol	1838.00		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/mol×K	586.72	Joback Method
cpg	186.29	J/mol×K	625.41	Joback Method
cpg	194.57	J/mol×K	664.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3393451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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