

2H-Pyran-3(4H)-one, dihydro-

Other names:	Dihydro-2H-pyran-3(4H)-one Tetrahydropyran-3-one 3-Tetrahydropyranone
Inchi:	InChI=1S/C5H8O2/c6-5-2-1-3-7-4-5/h1-4H2
InchiKey:	URUUZIAJVSGYRC-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	O=C1CCCOC1
Mol. weight [g/mol]:	100.12
CAS:	23462-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-185.33	kJ/mol	Joback Method
hf	-341.57	kJ/mol	Joback Method
hfus	6.96	kJ/mol	Joback Method
hvap	36.22	kJ/mol	Joback Method
log10ws	-0.18		Crippen Method
logp	0.366		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
ripol	1439.00		NIST Webbook
ripol	1439.00		NIST Webbook
tb	432.79	K	Joback Method
tc	662.42	K	Joback Method
tf	252.52	K	Joback Method
vc	0.278	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.33	J/molxK	432.79	Joback Method
cpg	163.57	J/molxK	471.06	Joback Method
cpg	175.28	J/molxK	509.33	Joback Method
cpg	186.47	J/molxK	547.60	Joback Method

cpg	197.12	J/mol×K	585.88	Joback Method
cpg	207.21	J/mol×K	624.15	Joback Method
cpg	216.74	J/mol×K	662.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23462751&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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