4H-Pyran-4-one, tetrahydro-

Other names:	Tetrahydro-«gamma»-pyrone
	Tetrahydro-4-pyrone
	Tetrahydro-4H-pyran-4-one
	2,3,5,6-Tetrahydro-4-pyranone
	4-Oxacyclohexanone
	4-Oxotetrahydropyran
Inchi:	InChI=1S/C5H8O2/c6-5-1-3-7-4-2-5/h1-4H2
InchiKey:	JMJRYTGVHCAYCT-UHFFFAOYSA-N
Formula:	C5H8O2
SMILES:	O=C1CCOCC1
Mol. weight [g/mol]:	100.12
CAS:	29943-42-8

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	50.70 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.18		Crippen Method
logp	0.366		Crippen Method
mcvol	77.890	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
tb	439.70	K	NIST Webbook
tc	662.42	K	Joback Method
tf	252.52	K	Joback Method
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	186.47	J/mol×K	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29943428&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

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