4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-

Other names: 3,5-Dihydroxy-6-methyl-2,3-dihydro-4H-pyran-4-one
2,3-dihydro-3,5-dihydroxy--6-methyl-4H-pyran-4-one
Pyranone
2,3-Dihydro-3,5-dihydroxy-6-methyl-4-pyrone
3-Hydroxy-2,3-dihydromaltol
3,5-Dihydroxy-2,3-dihydro-6-methyl-4-pyran-4-one, dihydroxy maltol
2,3-dihydro-3,5-dihydroxy-6-methyl-4(4H)-pyranone
2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyran-4-one (pyranone)
2,3-Dihydro-3,5-dihydroxy-6-methyl-4H-pyrene-4-one

Inchi: InChI=1S/C6H8O4/c1-3-5(8)6(9)4(7)2-10-3/h4,7-8H,2H2,1H3

InchiKey: VOLMSPGWNYJHQQ-UHFFFAOYSA-N

Formula: C6H8O4

SMILES: CC1=C(O)C(=O)C(O)CO1

Mol. weight [g/mol]: 144.13

CAS: 28564-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-447.56	kJ/mol	Joback Method
hf	-652.17	kJ/mol	Joback Method
hfus	19.24	kJ/mol	Joback Method
hvap	73.11	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.264		Crippen Method
mcvol	99.420	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
rinpol	1149.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1154.40		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1115.00		NIST Webbook

rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1154.40		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1144.00		NIST Webbook
ripol	2274.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2239.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2240.00		NIST Webbook
ripol	2229.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2300.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2311.00		NIST Webbook
ripol	2295.00		NIST Webbook
ripol	2267.00		NIST Webbook
ripol	2311.00		NIST Webbook
ripol	2275.00		NIST Webbook
ripol	2239.00		NIST Webbook
tb	644.48	K	Joback Method
tc	844.28	K	Joback Method
tf	406.99	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.35	J/mol×K	644.48	Joback Method
cpg	273.10	J/mol×K	677.78	Joback Method
cpg	281.42	J/mol×K	711.08	Joback Method
cpg	289.28	J/mol×K	744.38	Joback Method
cpg	296.67	J/mol×K	777.68	Joback Method
cpg	303.56	J/mol×K	810.98	Joback Method
cpg	309.95	J/mol×K	844.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28564832&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume