2,3-Dihydro-5-hydroxy-6-methyl-4(H)-pyran-4-one

Other names: 2,3-Dihydro-5-hydroxy-6-methyl-4H-pyran-4-one (dihydromaltol)
dihydromaltol
5-Hydroxy-6-methyl-2,3-dihydropyran-4-one (2,3-dihydromaltol)
Inchi: InChI=1S/C6H8O3/c1-4-6(8)5(7)2-3-9-4/h8H,2-3H2,1H3
InchiKey: YTKBKDDTNVNZLX-UHFFFAOYSA-N
Formula: C6H8O3
SMILES: CC1=C(O)C(=O)CCO1
Mol. weight [g/mol]: 128.13

Physical Properties

Property code	Value	Unit	Source
gf	-303.03	kJ/mol	Joback Method
hf	-479.60	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	56.74	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	0.765		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4876.56	kPa	Joback Method
rinpol	1066.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1104.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1868.00		NIST Webbook
ripol	1848.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1879.00		NIST Webbook
ripol	1860.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1848.00		NIST Webbook
tb	556.97	K	Joback Method
tc	771.16	K	Joback Method
tf	350.41	K	Joback Method

vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.38	J/mol×K	556.97	Joback Method
cpg	229.26	J/mol×K	592.67	Joback Method
cpg	238.71	J/mol×K	628.37	Joback Method
cpg	247.70	J/mol×K	664.06	Joback Method
cpg	256.23	J/mol×K	699.76	Joback Method
cpg	264.27	J/mol×K	735.46	Joback Method
cpg	271.82	J/mol×K	771.16	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R231042&Units=SI

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