4H-Pyran-4-one, 2,3-dihydro-3-hydroxy-6-methyl

Inchi: InChI=1S/C6H8O3/c1-4-2-5(7)6(8)3-9-4/h2,6,8H,3H2,1H3

InchiKey: FGIRKFUIPQCYJU-UHFFFAOYSA-N

Formula: C6H8O3

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

Mol. weight [g/mol]: 128.13

Physical Properties

Property code	Value	Unit	Source
gf	-301.11	kJ/mol	Joback Method
hf	-488.47	kJ/mol	Joback Method
hfus	15.54	kJ/mol	Joback Method
hvap	55.77	kJ/mol	Joback Method
log10ws	-0.32		Crippen Method
logp	-0.150		Crippen Method
mcvol	93.550	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
rinpol	1036.00		NIST Webbook
tb	547.32	K	Joback Method
tc	760.34	K	Joback Method
tf	333.65	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.31	J/mol×K	547.32	Joback Method
cpg	232.85	J/mol×K	582.82	Joback Method
cpg	242.91	J/mol×K	618.33	Joback Method
cpg	252.49	J/mol×K	653.83	Joback Method
cpg	261.56	J/mol×K	689.33	Joback Method
cpg	270.12	J/mol×K	724.84	Joback Method
cpg	278.13	J/mol×K	760.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R74672&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume