Pentanoic acid, 4-hydroxy-2-propyl, lactone, # 2

Inchi: InChI=1S/C8H14O2/c1-3-4-7-5-6(2)10-8(7)9/h6-7H,3-5H2,1-2H3
InchiKey: NMNZFIPBKPDLGC-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCCC1CC(C)OC1=O
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
gf	-163.39	kJ/mol	Joback Method
hf	-438.01	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	42.11	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.738		Crippen Method
mcvol	120.160	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1132.00		NIST Webbook
rinpol	1132.00		NIST Webbook
tb	487.82	K	Joback Method
tc	698.34	K	Joback Method
tf	281.37	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.47	J/mol×K	487.82	Joback Method
cpg	294.24	J/mol×K	522.91	Joback Method
cpg	309.36	J/mol×K	557.99	Joback Method
cpg	323.81	J/mol×K	593.08	Joback Method
cpg	337.60	J/mol×K	628.17	Joback Method
cpg	350.70	J/mol×K	663.26	Joback Method
cpg	363.12	J/mol×K	698.34	Joback Method

Sources

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=R167996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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