5-Hydroxy-3,4-dimethyl-5-pentyl-2(5H)-furanone

Inchi: InChI=1S/C11H18O3/c1-4-5-6-7-11(13)9(3)8(2)10(12)14-11/h13H,4-7H2,1-3H3
InchiKey: VJZWZDQDXPADSE-UHFFFAOYSA-N
Formula: C11H18O3
SMILES: CCCCCC1(O)OC(=O)C(C)=C1C
Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
gf	-262.03	kJ/mol	Joback Method
hf	-581.74	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	66.24	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.149		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
ripol	2710.00		NIST Webbook
ripol	2710.00		NIST Webbook
tb	662.67	K	Joback Method
tc	862.15	K	Joback Method
tf	429.94	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.06	J/mol×K	662.67	Joback Method
cpg	469.57	J/mol×K	695.92	Joback Method
cpg	482.56	J/mol×K	729.16	Joback Method
cpg	495.10	J/mol×K	762.41	Joback Method
cpg	507.25	J/mol×K	795.66	Joback Method

cpg	519.08	J/mol×K	828.90	Joback Method
cpg	530.66	J/mol×K	862.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326244&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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