2,5-Dimethyl-4-(3-hexenoyl)-3(3H)furanone

Other names: 3(2H)-Furanone, 2,5-dimethyl-4-[(Z)-3-hexenyloxy]
Inchi: InChI=1S/C12H18O3/c1-4-5-6-7-8-14-12-10(3)15-9(2)11(12)13/h5-6,9H,4,7-8H2,1-3H3/b
InchiKey: MMUPBVLKMLEXCF-AATRIKPKSA-N
Formula: C12H18O3
SMILES: CCC=CCCOC1=C(C)OC(C)C1=O
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-136.08	kJ/mol	Joback Method
hf	-480.39	kJ/mol	Joback Method
hfus	30.09	kJ/mol	Joback Method
hvap	55.30	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.579		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	1480.00		NIST Webbook
tb	619.71	K	Joback Method
tc	828.25	K	Joback Method
tf	373.64	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.57	J/mol×K	619.71	Joback Method
cpg	472.84	J/mol×K	654.47	Joback Method
cpg	488.31	J/mol×K	689.22	Joback Method
cpg	502.98	J/mol×K	723.98	Joback Method
cpg	516.85	J/mol×K	758.74	Joback Method
cpg	529.91	J/mol×K	793.49	Joback Method
cpg	542.17	J/mol×K	828.25	Joback Method

Sources

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=U322345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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