3(2H)-Furanone, 2-hexyl-5-methyl-

Other names:	2-Hexyl-5-methyl-3(2H)-furanone
	2,3-Dihydro-2-n-hexyl-5-methyl-furan-3-one
	2,3-Dihydro-5-methyl-2-n-hexylfuran-3-one
	2-Hexyl-5-methyl-2(3H)-furan-3-one
	2-Hexyl-5-methyl-(2H)-furan-3-one
Inchi:	InChI=1S/C11H18O2/c1-3-4-5-6-7-11-10(12)8-9(2)13-11/h8,11H,3-7H2,1-2H3
InchiKey:	AAUWBAWSKVOBFL-UHFFFAOYSA-N
Formula:	C11H18O2
SMILES:	CCCCCCC1OC(C)=CC1=O
Mol. weight [g/mol]:	182.26
CAS:	33922-66-6

Physical Properties

Property code	Value	Unit	Source
gf	-110.09	kJ/mol	Joback Method
hf	-433.28	kJ/mol	Joback Method
hfus	26.50	kJ/mol	Joback Method
hvap	50.05	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.828		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1446.10		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1446.10		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	1999.00		NIST Webbook
tb	565.27	K	Joback Method
tc	769.60	K	Joback Method
tf	332.70	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.06	J/mol×K	565.27	Joback Method
cpg	416.63	J/mol×K	599.33	Joback Method
cpg	432.42	J/mol×K	633.38	Joback Method
cpg	447.44	J/mol×K	667.44	Joback Method
cpg	461.70	J/mol×K	701.49	Joback Method
cpg	475.19	J/mol×K	735.55	Joback Method
cpg	487.92	J/mol×K	769.60	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=C33922666&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