3,4-Dimethyl-5-pentyl-5H-furan-2-one

Other names: 2,3-Dimethyl-2-nonen-4-olide
Inchi: InChI=1S/C11H18O2/c1-4-5-6-7-10-8(2)9(3)11(12)13-10/h10H,4-7H2,1-3H3
InchiKey: LRKURLXWGJNWOJ-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: CCCCCC1OC(=O)C(C)=C1C
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-119.72	kJ/mol	Joback Method
hf	-444.75	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	50.71	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.828		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
ripol	2195.00		NIST Webbook
ripol	2206.00		NIST Webbook
tb	570.25	K	Joback Method
tc	775.60	K	Joback Method
tf	345.22	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.09	J/mol×K	570.25	Joback Method
cpg	416.40	J/mol×K	604.47	Joback Method
cpg	431.99	J/mol×K	638.70	Joback Method
cpg	446.83	J/mol×K	672.92	Joback Method
cpg	460.95	J/mol×K	707.15	Joback Method
cpg	474.33	J/mol×K	741.37	Joback Method
cpg	486.96	J/mol×K	775.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R425673&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume