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

Other names:	bovolide
	2(5H)-Furanone, 3,4-dimethyl-5-pentylidene-
Inchi:	InChI=1S/C11H16O2/c1-4-5-6-7-10-8(2)9(3)11(12)13-10/h7H,4-6H2,1-3H3/b10-7+
InchiKey:	MTQPZHNZYWAXEH-JXMROGBWSA-N
Formula:	C11H16O2
SMILES:	CCCCC=C1OC(=O)C(C)=C1C
Mol. weight [g/mol]:	180.24
CAS:	774-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-66.55	kJ/mol	Joback Method
hf	-348.38	kJ/mol	Joback Method
hfus	25.37	kJ/mol	Joback Method
hvap	51.81	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.954		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
ripol	2179.00		NIST Webbook
ripol	2170.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2191.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
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ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2170.00		NIST Webbook

ripol	2174.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
tb	581.56	K	Joback Method
tc	793.40	K	Joback Method
tf	359.82	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.70	J/mol×K	581.56	Joback Method
cpg	393.57	J/mol×K	616.87	Joback Method
cpg	407.72	J/mol×K	652.17	Joback Method
cpg	421.18	J/mol×K	687.48	Joback Method
cpg	433.95	J/mol×K	722.79	Joback Method
cpg	446.03	J/mol×K	758.09	Joback Method
cpg	457.43	J/mol×K	793.40	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=C774641&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume