dihydrobovolide

Other names: 3,4-dimetthyl-5-pentylidene-2(5H)-furanone
Inchi: InChI=1S/C11H18O2/c1-4-5-6-7-10-8(2)9(3)11(12)13-10/h7-9H,4-6H2,1-3H3/b10-7+
InchiKey: GKHOOSNEXYJMQR-JXMROGBWSA-N
Formula: C11H18O2
SMILES: CCCCC=C1OC(=O)C(C)C1C
Mol. weight [g/mol]: 182.26
CAS: 51352-68-2

Physical Properties

Property code	Value	Unit	Source
gf	-92.67	kJ/mol	Joback Method
hf	-423.90	kJ/mol	Joback Method
hfus	27.06	kJ/mol	Joback Method
hvap	49.57	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.889		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
ripol	2179.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2131.00		NIST Webbook
ripol	2131.00		NIST Webbook
tb	563.10	K	Joback Method
tc	770.79	K	Joback Method
tf	325.54	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.50	J/mol×K	563.10	Joback Method
cpg	418.84	J/mol×K	597.72	Joback Method
cpg	435.37	J/mol×K	632.33	Joback Method
cpg	451.09	J/mol×K	666.95	Joback Method

cpg	466.00	J/mol×K	701.56	Joback Method
cpg	480.11	J/mol×K	736.18	Joback Method
cpg	493.41	J/mol×K	770.79	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=C51352682&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume