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

Other names: 3(2H)-Furanone, 2,5-dimethyl-4-(3-methylbutoxy)
Inchi: InChI=1S/C11H18O3/c1-7(2)5-6-13-11-9(4)14-8(3)10(11)12/h7-8H,5-6H2,1-4H3
InchiKey: ATDNOZAARFGQGA-UHFFFAOYSA-N
Formula: C11H18O3
SMILES: CC1=C(OCCC(C)C)C(=O)C(C)O1
Mol. weight [g/mol]: 198.26

Physical Properties

Property code	Value	Unit	Source
gf	-227.16	kJ/mol	Joback Method
hf	-582.25	kJ/mol	Joback Method
hfus	23.78	kJ/mol	Joback Method
hvap	52.73	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.268		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	592.23	K	Joback Method
tc	799.69	K	Joback Method
tf	352.45	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.87	J/mol×K	592.23	Joback Method
cpg	443.30	J/mol×K	626.81	Joback Method
cpg	459.00	J/mol×K	661.38	Joback Method
cpg	473.94	J/mol×K	695.96	Joback Method
cpg	488.11	J/mol×K	730.54	Joback Method
cpg	501.50	J/mol×K	765.11	Joback Method
cpg	514.09	J/mol×K	799.69	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=U322344&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume