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

Other names: 3(2H)-Furanone, 2,5-dimethyl-4-butoxy
Inchi: InChI=1S/C10H16O3/c1-4-5-6-12-10-8(3)13-7(2)9(10)11/h7H,4-6H2,1-3H3
InchiKey: SQHHYGNRSINKBH-UHFFFAOYSA-N
Formula: C10H16O3
SMILES: CCCCOC1=C(C)OC(C)C1=O
Mol. weight [g/mol]: 184.23

Physical Properties

Property code	Value	Unit	Source
gf	-233.14	kJ/mol	Joback Method
hf	-556.33	kJ/mol	Joback Method
hfus	24.71	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.022		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	569.79	K	Joback Method
tc	776.24	K	Joback Method
tf	356.18	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.50	J/mol×K	569.79	Joback Method
cpg	392.77	J/mol×K	604.20	Joback Method
cpg	407.41	J/mol×K	638.61	Joback Method
cpg	421.40	J/mol×K	673.02	Joback Method
cpg	434.71	J/mol×K	707.43	Joback Method
cpg	447.34	J/mol×K	741.83	Joback Method
cpg	459.27	J/mol×K	776.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U322343&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume