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

Other names: 3(2H)-Furanone, 2,5-dimethyl-4-ethoxy
Inchi: InChI=1S/C8H12O3/c1-4-10-8-6(3)11-5(2)7(8)9/h5H,4H2,1-3H3
InchiKey: AILFSZXBRNLVHY-UHFFFAOYSA-N
Formula: C8H12O3
SMILES: CCOC1=C(C)OC(C)C1=O
Mol. weight [g/mol]: 156.18

Physical Properties

Property code	Value	Unit	Source
gf	-249.98	kJ/mol	Joback Method
hf	-515.05	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.242		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
tb	524.03	K	Joback Method
tc	737.18	K	Joback Method
tf	333.64	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.94	J/mol×K	524.03	Joback Method
cpg	298.23	J/mol×K	559.56	Joback Method
cpg	311.05	J/mol×K	595.08	Joback Method
cpg	323.36	J/mol×K	630.61	Joback Method
cpg	335.15	J/mol×K	666.13	Joback Method
cpg	346.38	J/mol×K	701.66	Joback Method
cpg	357.02	J/mol×K	737.18	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=U322342&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume