5-Methyl-2-octyl-[2 H]-furan-3-one

Inchi: InChI=1S/C13H24O2/c1-3-4-5-6-7-8-9-13-12(14)10-11(2)15-13/h11,13H,3-10H2,1-2H3
InchiKey: HHRJNMXGPAQRLS-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CCCCCCCCC1OC(C)CC1=O
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-121.29	kJ/mol	Joback Method
hf	-541.21	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.483		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
ripol	2193.00		NIST Webbook
ripol	2193.00		NIST Webbook
tb	602.22	K	Joback Method
tc	798.06	K	Joback Method
tf	337.72	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.33	J/mol×K	602.22	Joback Method
cpg	542.76	J/mol×K	634.86	Joback Method
cpg	561.26	J/mol×K	667.50	Joback Method
cpg	578.85	J/mol×K	700.14	Joback Method
cpg	595.52	J/mol×K	732.78	Joback Method
cpg	611.29	J/mol×K	765.42	Joback Method
cpg	626.16	J/mol×K	798.06	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=R422867&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