2,3-dihydro-2-decyl-5-methylfuran-3-one

Inchi: InChI=1S/C15H26O2/c1-3-4-5-6-7-8-9-10-11-15-14(16)12-13(2)17-15/h12,15H,3-11H2,1
InchiKey: KMBDEJFSHYHVTJ-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CCCCCCCCCCC1OC(C)=CC1=O
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-76.41	kJ/mol	Joback Method
hf	-515.84	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.389		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1838.00		NIST Webbook
tb	656.79	K	Joback Method
tc	850.59	K	Joback Method
tf	377.78	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.39	J/mol×K	656.79	Joback Method
cpg	627.06	J/mol×K	689.09	Joback Method
cpg	644.80	J/mol×K	721.39	Joback Method
cpg	661.61	J/mol×K	753.69	Joback Method
cpg	677.51	J/mol×K	785.99	Joback Method
cpg	692.51	J/mol×K	818.29	Joback Method
cpg	706.63	J/mol×K	850.59	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=R220601&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