dihydro-4-methyl-5-pentylfuran-2(3H)-one

Other names: 4-Methyl-5-pentyldihydrofuran-2(3H)-one
Inchi: InChI=1S/C10H18O2/c1-3-4-5-6-9-8(2)7-10(11)12-9/h8-9H,3-7H2,1-2H3
InchiKey: LOQFOBUZYRBURV-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCCCC1OC(=O)CC1C
Mol. weight [g/mol]: 170.25
CAS: 33673-62-0

Physical Properties

Property code	Value	Unit	Source
gf	-146.55	kJ/mol	Joback Method
hf	-479.29	kJ/mol	Joback Method
hfus	24.15	kJ/mol	Joback Method
hvap	46.56	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.518		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinpol	1501.80		NIST Webbook
rinpol	1501.80		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2070.00		NIST Webbook
tb	533.58	K	Joback Method
tc	737.90	K	Joback Method
tf	303.91	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.11	J/mol×K	533.58	Joback Method
cpg	388.73	J/mol×K	567.63	Joback Method
cpg	405.55	J/mol×K	601.69	Joback Method
cpg	421.59	J/mol×K	635.74	Joback Method

cpg	436.85	J/mol×K	669.79	Joback Method
cpg	451.32	J/mol×K	703.84	Joback Method
cpg	465.00	J/mol×K	737.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33673620&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume