5-[(E)-Hexylidene]-5H-furan-2-one

Inchi: InChI=1S/C9H12O2/c1-2-3-4-5-8-6-7-9(10)11-8/h5-7H,2-4H2,1H3/b8-5+
InchiKey: ICHISWQVYXYNPA-VMPITWQZSA-N
Formula: C9H12O2
SMILES: CCCCC=C1C=CC(=O)O1
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
gf	-64.13	kJ/mol	Joback Method
hf	-284.16	kJ/mol	Joback Method
hfus	20.96	kJ/mol	Joback Method
hvap	46.03	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.173		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1424.00		NIST Webbook
rinpol	1424.00		NIST Webbook
ripol	2211.00		NIST Webbook
ripol	2211.00		NIST Webbook
tb	525.84	K	Joback Method
tc	742.74	K	Joback Method
tf	312.24	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.46	J/mol×K	525.84	Joback Method
cpg	300.09	J/mol×K	561.99	Joback Method
cpg	313.02	J/mol×K	598.14	Joback Method
cpg	325.26	J/mol×K	634.29	Joback Method
cpg	336.84	J/mol×K	670.44	Joback Method
cpg	347.75	J/mol×K	706.59	Joback Method

cpg	358.03	J/mol×K	742.74	Joback Method

Sources

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=R411882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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