5-Pentyl-3H-furan-2-one

Other names: 5-Pentyl-2(3H)-furanone
Inchi: InChI=1S/C9H14O2/c1-2-3-4-5-8-6-7-9(10)11-8/h6H,2-5,7H2,1H3
InchiKey: PGAMJXWVUGDLRA-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CCCCCC1=CCC(=O)O1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-119.22	kJ/mol	Joback Method
hf	-371.66	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	45.91	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.397		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1273.00		NIST Webbook
tb	524.18	K	Joback Method
tc	735.12	K	Joback Method
tf	314.40	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.50	J/mol×K	524.18	Joback Method
cpg	318.98	J/mol×K	559.34	Joback Method
cpg	332.79	J/mol×K	594.49	Joback Method
cpg	345.91	J/mol×K	629.65	Joback Method

cpg	358.37	J/mol×K	664.80	Joback Method
cpg	370.17	J/mol×K	699.96	Joback Method
cpg	381.30	J/mol×K	735.12	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=R406281&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