5-Butyl-2(5H)-furanone

Inchi: InChI=1S/C8H12O2/c1-2-3-4-7-5-6-8(9)10-7/h5-7H,2-4H2,1H3
InchiKey: KGJZBUMJSZTLTA-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CCCCC1C=CC(=O)O1
Mol. weight [g/mol]: 140.18

Physical Properties

Property code	Value	Unit	Source
gf	-125.72	kJ/mol	Joback Method
hf	-359.89	kJ/mol	Joback Method
hfus	19.12	kJ/mol	Joback Method
hvap	42.71	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.658		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
ripol	1937.00		NIST Webbook
ripol	1937.00		NIST Webbook
tb	491.65	K	Joback Method
tc	704.52	K	Joback Method
tf	286.37	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.08	J/mol×K	491.65	Joback Method
cpg	275.26	J/mol×K	527.13	Joback Method
cpg	288.79	J/mol×K	562.61	Joback Method
cpg	301.67	J/mol×K	598.09	Joback Method
cpg	313.90	J/mol×K	633.56	Joback Method
cpg	325.49	J/mol×K	669.04	Joback Method
cpg	336.42	J/mol×K	704.52	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=R569263&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume