2(5H)-Furanone, 5-chloromethyl-3-methyl

Inchi: InChI=1S/C6H7ClO2/c1-4-2-5(3-7)9-6(4)8/h2,5H,3H2,1H3
InchiKey: RWOREBHQQOTRGU-UHFFFAOYSA-N
Formula: C6H7ClO2
SMILES: CC1=CC(CCl)OC1=O
Mol. weight [g/mol]: 146.57

Physical Properties

Property code	Value	Unit	Source
gf	-164.12	kJ/mol	Joback Method
hf	-345.82	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	43.30	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.097		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	1193.00		NIST Webbook
tb	488.30	K	Joback Method
tc	715.17	K	Joback Method
tf	306.27	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.65	J/mol×K	488.30	Joback Method
cpg	213.43	J/mol×K	526.11	Joback Method
cpg	223.74	J/mol×K	563.92	Joback Method
cpg	233.56	J/mol×K	601.73	Joback Method
cpg	242.88	J/mol×K	639.55	Joback Method
cpg	251.70	J/mol×K	677.36	Joback Method
cpg	260.00	J/mol×K	715.17	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=R508679&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume