3(2H)-Furanone, dihydro

Other names: Oxolan-3-one
Inchi: InChI=1S/C4H6O2/c5-4-1-2-6-3-4/h1-3H2
InchiKey: JLPJFSCQKHRSQR-UHFFFAOYSA-N
Formula: C4H6O2
SMILES: O=C1CCOC1
Mol. weight [g/mol]: 86.09

Physical Properties

Property code	Value	Unit	Source
gf	-181.65	kJ/mol	Joback Method
hf	-314.77	kJ/mol	Joback Method
hfus	6.47	kJ/mol	Joback Method
hvap	33.82	kJ/mol	Joback Method
log10ws	0.24		Crippen Method
logp	-0.024		Crippen Method
mcvol	63.800	ml/mol	McGowan Method
pc	5382.80	kPa	Joback Method
rinpol	715.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	694.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	694.00		NIST Webbook
tb	405.64	K	Joback Method
tc	628.74	K	Joback Method
tf	244.77	K	Joback Method
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.24	J/mol×K	405.64	Joback Method
cpg	125.93	J/mol×K	442.82	Joback Method
cpg	135.22	J/mol×K	480.01	Joback Method
cpg	144.12	J/mol×K	517.19	Joback Method

cpg	152.61	J/mol×K	554.37	Joback Method
cpg	160.69	J/mol×K	591.56	Joback Method
cpg	168.36	J/mol×K	628.74	Joback Method

Sources

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=R69685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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