3,4,5-trimethyl-2[5H]-furanon

Inchi: InChI=1S/C7H10O2/c1-4-5(2)7(8)9-6(4)3/h6H,1-3H3
InchiKey: OSFZDFIHIYXIEL-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC1=C(C)C(C)OC1=O
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
gf	-153.40	kJ/mol	Joback Method
hf	-362.19	kJ/mol	Joback Method
hfus	15.75	kJ/mol	Joback Method
hvap	41.81	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.268		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
ripol	1822.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1822.00		NIST Webbook
tb	478.73	K	Joback Method
tc	697.51	K	Joback Method
tf	300.14	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.26	J/mol×K	478.73	Joback Method
cpg	231.43	J/mol×K	515.19	Joback Method
cpg	243.16	J/mol×K	551.66	Joback Method
cpg	254.43	J/mol×K	588.12	Joback Method
cpg	265.23	J/mol×K	624.58	Joback Method
cpg	275.54	J/mol×K	661.05	Joback Method

cpg	285.34	J/mol×K	697.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R491551&Units=SI
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

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