2,5-dimethyl-3(2H)-furanone

Other names: 2H-Furan-3-one, 2,5-dimethyl
3(2H)-Furanone, 2,5-dimethyl-
2,5-dimethylfuran-3(2H)-one
Inchi: InChI=1S/C6H8O2/c1-4-3-6(7)5(2)8-4/h3,5H,1-2H3
InchiKey: ASOSVCXGWPDUGN-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1=CC(=O)C(C)O1
Mol. weight [g/mol]: 112.13
CAS: 14400-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-152.19	kJ/mol	Joback Method
hf	-330.08	kJ/mol	Joback Method
hfus	13.55	kJ/mol	Joback Method
hvap	38.92	kJ/mol	Joback Method
ie	9.23 ± 0.05	eV	NIST Webbook
log10ws	-1.06		Crippen Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	917.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1492.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1518.00		NIST Webbook
ripol	1493.00		NIST Webbook
tb	450.87	K	Joback Method
tc	671.60	K	Joback Method

tf	276.35	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.89	J/mol×K	450.87	Joback Method
cpg	190.07	J/mol×K	487.66	Joback Method
cpg	200.83	J/mol×K	524.45	Joback Method
cpg	211.16	J/mol×K	561.23	Joback Method
cpg	221.04	J/mol×K	598.02	Joback Method
cpg	230.47	J/mol×K	634.81	Joback Method
cpg	239.42	J/mol×K	671.60	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=C14400670&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
ie: Ionization energy
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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume