2,2-DIMETHYL-3(2H)-FURANONE

Inchi: InChI=1S/C6H8O2/c1-6(2)5(7)3-4-8-6/h3-4H,1-2H3
InchiKey: HVNICCSXGONRCB-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: CC1(C)OC=CC1=O
Mol. weight [g/mol]: 112.13

Physical Properties

Property code	Value	Unit	Source
hfus	7.64	kJ/mol	Joback Method
logp	0.878		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
rinpol	834.00		NIST Webbook
rinpol	834.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.23	J/mol×K	446.13	Joback Method
cpg	191.02	J/mol×K	484.37	Joback Method
cpg	201.97	J/mol×K	522.61	Joback Method
cpg	212.19	J/mol×K	560.84	Joback Method
cpg	221.76	J/mol×K	599.08	Joback Method
cpg	230.78	J/mol×K	637.32	Joback Method
cpg	239.35	J/mol×K	675.56	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35298487&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices