2(5H)-FURANONE, 5-(1-METHYLETHYL)-

Other names: 5-Isopropyl-5H-furan-2-one
Inchi: InChI=1S/C7H10O2/c1-5(2)6-3-4-7(8)9-6/h3-6H,1-2H3
InchiKey: LWFKYUIZWLTJCA-UHFFFAOYSA-N
Formula: C7H10O2
SMILES: CC(C)C1C=CC(=O)O1
Mol. weight [g/mol]: 126.15

Physical Properties

Property code	Value	Unit	Source
hfus	13.01	kJ/mol	Joback Method
ie	10.30	eV	Cheméo Relay (1.0)
logp	1.124		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
rinpol	1311.00		NIST Webbook
rinpol	1311.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.87	J/mol×K	468.33	Joback Method
cpg	232.27	J/mol×K	505.22	Joback Method
cpg	245.06	J/mol×K	542.10	Joback Method
cpg	257.22	J/mol×K	578.99	Joback Method
cpg	268.77	J/mol×K	615.87	Joback Method
cpg	279.69	J/mol×K	652.76	Joback Method
cpg	289.99	J/mol×K	689.64	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56767192&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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