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

Other names: Butyric acid, 2,2-dimethyl-4-hydroxy-, g-lactone
Inchi: InChI=1S/C6H10O2/c1-6(2)3-4-8-5(6)7/h3-4H2,1-2H3
InchiKey: UPVAIJPDWVTFKT-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CC1(C)CCOC1=O
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
hf	-383.27	kJ/mol	Cheméo Relay (1.0)
hfus	6.42	kJ/mol	Joback Method
hvap	45.62	kJ/mol	Cheméo Relay (1.0)
ie	9.82	eV	Cheméo Relay (1.0)
logp	0.960		Crippen Method
mcvol	91.980	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.83	J/mol×K	446.97	Joback Method
cpg	207.04	J/mol×K	484.80	Joback Method
cpg	219.39	J/mol×K	522.63	Joback Method
cpg	230.96	J/mol×K	560.45	Joback Method
cpg	241.84	J/mol×K	598.28	Joback Method
cpg	252.12	J/mol×K	636.11	Joback Method
cpg	261.89	J/mol×K	673.94	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3709088&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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume