1,3-Cyclohexanedione, 4,4-dimethyl-

Inchi: InChI=1S/C8H12O2/c1-8(2)4-3-6(9)5-7(8)10/h3-5H2,1-2H3
InchiKey: PLGPBTCNKJQJHQ-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CC1(C)CCC(=O)CC1=O
Mol. weight [g/mol]: 140.18
CAS: 562-46-9

Physical Properties

Property code	Value	Unit	Source
chs	-4363.50 ± 1.30	kJ/mol	NIST Webbook
gf	-209.74	kJ/mol	Joback Method
hf	-400.40 ± 2.70	kJ/mol	NIST Webbook
hfs	-499.60 ± 1.70	kJ/mol	NIST Webbook
hfus	1.03	kJ/mol	Joback Method
hsub	99.20 ± 2.10	kJ/mol	NIST Webbook
hsub	99.20 ± 2.10	kJ/mol	NIST Webbook
hvap	41.17	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.335		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	537.87	K	Joback Method
tc	785.42	K	Joback Method
tf	347.64	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.77	J/mol×K	537.87	Joback Method
cpg	292.13	J/mol×K	579.13	Joback Method
cpg	307.63	J/mol×K	620.39	Joback Method
cpg	322.36	J/mol×K	661.64	Joback Method
cpg	336.38	J/mol×K	702.90	Joback Method

cpg	349.76	J/mol×K	744.16	Joback Method
cpg	362.57	J/mol×K	785.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.20	K	0.90	NIST Webbook

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=C562469&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume