1,2-Cyclopentanedione, 3,4,4-trimethyl-

Other names: 3,4,4-trimethylcyclopentane-1,2-dione
Inchi: InChI=1S/C8H12O2/c1-5-7(10)6(9)4-8(5,2)3/h5H,4H2,1-3H3
InchiKey: YHJBEOWTWJHMFC-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CC1C(=O)C(=O)CC1(C)C
Mol. weight [g/mol]: 140.18
CAS: 33079-56-0

Physical Properties

Property code	Value	Unit	Source
gf	-205.35	kJ/mol	Joback Method
hf	-428.47	kJ/mol	Joback Method
hfus	4.20	kJ/mol	Joback Method
hvap	40.69	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.191		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1088.00		NIST Webbook
tb	528.93	K	Joback Method
tc	767.28	K	Joback Method
tf	346.92	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.01	J/mol×K	528.93	Joback Method
cpg	292.74	J/mol×K	568.65	Joback Method
cpg	307.71	J/mol×K	608.38	Joback Method
cpg	321.97	J/mol×K	648.10	Joback Method
cpg	335.60	J/mol×K	687.83	Joback Method
cpg	348.65	J/mol×K	727.55	Joback Method
cpg	361.18	J/mol×K	767.28	Joback Method

Sources

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=C33079560&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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