Cyclopentanecarboxylic acid, 3-oxo-, methyl ester

Other names: Methyl 3-oxocyclopentanecarboxylate
3-Carbomethoxycyclopentanone
Inchi: InChI=1S/C7H10O3/c1-10-7(9)5-2-3-6(8)4-5/h5H,2-4H2,1H3
InchiKey: KTGCFXSELRVRFH-UHFFFAOYSA-N
Formula: C7H10O3
SMILES: COC(=O)C1CCC(=O)C1
Mol. weight [g/mol]: 142.15
CAS: 32811-75-9

Physical Properties

Property code	Value	Unit	Source
gf	-311.90	kJ/mol	Joback Method
hf	-509.83	kJ/mol	Joback Method
hfus	10.12	kJ/mol	Joback Method
hvap	44.84	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.529		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
tb	518.95	K	Joback Method
tc	742.25	K	Joback Method
tf	319.93	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.16	J/mol×K	518.95	Joback Method
cpg	260.76	J/mol×K	556.17	Joback Method
cpg	273.75	J/mol×K	593.38	Joback Method
cpg	286.12	J/mol×K	630.60	Joback Method
cpg	297.83	J/mol×K	667.82	Joback Method
cpg	308.88	J/mol×K	705.03	Joback Method
cpg	319.24	J/mol×K	742.25	Joback Method

Sources

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=C32811759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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