3-Methyl-2-methoxycarbonylcyclopentanone

Inchi: InChI=1S/C9H14O3/c1-3-12-9(11)8-6(2)4-5-7(8)10/h6,8H,3-5H2,1-2H3
InchiKey: LPGXYGZNLBXGSA-UHFFFAOYSA-N
Formula: C9H14O3
SMILES: CCOC(=O)C1C(=O)CCC1C
Mol. weight [g/mol]: 170.21
CAS: 58073-90-8

Physical Properties

Property code	Value	Unit	Source
gf	-302.77	kJ/mol	Joback Method
hf	-571.45	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	1.165		Crippen Method
mcvol	135.820	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1238.00		NIST Webbook
rinpol	1238.00		NIST Webbook
tb	560.04	K	Joback Method
tc	775.61	K	Joback Method
tf	338.23	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.32	J/mol×K	560.04	Joback Method
cpg	356.31	J/mol×K	595.97	Joback Method
cpg	371.55	J/mol×K	631.90	Joback Method
cpg	386.03	J/mol×K	667.82	Joback Method
cpg	399.73	J/mol×K	703.75	Joback Method
cpg	412.62	J/mol×K	739.68	Joback Method
cpg	424.69	J/mol×K	775.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58073908&Units=SI
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

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