3-(Methoxycarbonyl)-3-cyclooctenone

Inchi: InChI=1S/C10H14O3/c1-13-10(12)8-5-3-2-4-6-9(11)7-8/h7H,2-6H2,1H3/b8-7+
InchiKey: HVNCTECESWBWRG-BQYQJAHWSA-N
Formula: C10H14O3
SMILES: COC(=O)C1=CC(=O)CCCCC1
Mol. weight [g/mol]: 182.22
CAS: 17606-95-0

Physical Properties

Property code	Value	Unit	Source
gf	-294.90	kJ/mol	Joback Method
hf	-523.58	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	53.29	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.619		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	609.21	K	Joback Method
tc	847.27	K	Joback Method
tf	360.70	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.62	J/mol×K	609.21	Joback Method
cpg	385.95	J/mol×K	648.89	Joback Method
cpg	402.24	J/mol×K	688.56	Joback Method
cpg	417.46	J/mol×K	728.24	Joback Method
cpg	431.57	J/mol×K	767.92	Joback Method
cpg	444.51	J/mol×K	807.60	Joback Method
cpg	456.26	J/mol×K	847.27	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=C17606950&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