2-Cyclopenten-1-one, 4-methoxy-

Inchi: InChI=1S/C6H8O2/c1-8-6-3-2-5(7)4-6/h2-3,6H,4H2,1H3
InchiKey: FXNNWSRLQNFYQI-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: COC1C=CC(=O)C1
Mol. weight [g/mol]: 112.13
CAS: 61322-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-161.44	kJ/mol	Joback Method
hf	-318.83	kJ/mol	Joback Method
hfus	7.15	kJ/mol	Joback Method
hvap	36.16	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.530		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	441.36	K	Joback Method
tc	659.84	K	Joback Method
tf	259.49	K	Joback Method
vc	0.324	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.53	J/mol×K	441.36	Joback Method
cpg	185.19	J/mol×K	477.77	Joback Method
cpg	196.45	J/mol×K	514.19	Joback Method
cpg	207.27	J/mol×K	550.60	Joback Method
cpg	217.66	J/mol×K	587.01	Joback Method
cpg	227.58	J/mol×K	623.43	Joback Method
cpg	237.01	J/mol×K	659.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61322972&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume