2-Ethyl-3-methoxy-2-cyclopentenone

Inchi: InChI=1S/C8H12O2/c1-3-6-7(9)4-5-8(6)10-2/h3-5H2,1-2H3
InchiKey: CGBUGQQOHMWSAF-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: CCC1=C(OC)CCC1=O
Mol. weight [g/mol]: 140.18
CAS: 25112-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-156.15	kJ/mol	Joback Method
hf	-362.71	kJ/mol	Joback Method
hfus	10.48	kJ/mol	Joback Method
hvap	42.24	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.660		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	501.75	K	Joback Method
tc	716.67	K	Joback Method
tf	311.31	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.12	J/mol×K	501.75	Joback Method
cpg	268.35	J/mol×K	537.57	Joback Method
cpg	281.10	J/mol×K	573.39	Joback Method
cpg	293.33	J/mol×K	609.21	Joback Method
cpg	305.04	J/mol×K	645.03	Joback Method
cpg	316.20	J/mol×K	680.85	Joback Method
cpg	326.80	J/mol×K	716.67	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=C25112861&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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