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

Physical Properties

Property code	Value	Unit	Source
hfus	10.48	kJ/mol	Joback Method
logp	1.660		Crippen Method
mcvol	115.860	ml/mol	McGowan 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25112861&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume