2-Ethyl-3,5-dimethyl-2-cyclopenten-1-one

Inchi: InChI=1S/C9H14O/c1-4-8-6(2)5-7(3)9(8)10/h7H,4-5H2,1-3H3
InchiKey: LQDRSCFEBFOVPB-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CCC1=C(C)CC(C)C1=O
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	-50.44	kJ/mol	Joback Method
hf	-271.47	kJ/mol	Joback Method
hfus	12.96	kJ/mol	Joback Method
hvap	41.75	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1120.00		NIST Webbook
ripol	1506.00		NIST Webbook
tb	497.54	K	Joback Method
tc	711.00	K	Joback Method
tf	296.11	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.11	J/mol×K	497.54	Joback Method
cpg	291.06	J/mol×K	533.12	Joback Method
cpg	305.40	J/mol×K	568.69	Joback Method
cpg	319.13	J/mol×K	604.27	Joback Method
cpg	332.24	J/mol×K	639.85	Joback Method
cpg	344.72	J/mol×K	675.42	Joback Method
cpg	356.58	J/mol×K	711.00	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=R416223&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume