2-Cyclohexen-1-one, 4-ethyl-3,4-dimethyl-

Other names: 4-Ethyl-3,4-dimethyl-2-cyclohexen-1-one
Inchi: InChI=1S/C10H16O/c1-4-10(3)6-5-9(11)7-8(10)2/h7H,4-6H2,1-3H3
InchiKey: LVBPXRKIGDMCEV-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CCC1(C)CCC(=O)C=C1C
Mol. weight [g/mol]: 152.23
CAS: 17622-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-49.98	kJ/mol	Joback Method
hf	-271.56	kJ/mol	Joback Method
hfus	7.54	kJ/mol	Joback Method
hvap	42.33	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.712		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1150.00		NIST Webbook
tb	519.95	K	Joback Method
tc	746.03	K	Joback Method
tf	315.24	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.97	J/mol×K	519.95	Joback Method
cpg	338.18	J/mol×K	557.63	Joback Method
cpg	354.42	J/mol×K	595.31	Joback Method
cpg	369.79	J/mol×K	632.99	Joback Method
cpg	384.38	J/mol×K	670.67	Joback Method
cpg	398.28	J/mol×K	708.35	Joback Method
cpg	411.58	J/mol×K	746.03	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=C17622467&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume