2-Cyclohexen-1-one, 3-ethoxy-5,5-dimethyl-

Other names: 3-Ethoxy-5,5-dimethyl-cyclohex-2-enone
3-Ethoxy-5,5-dimethyl-2-cyclohexen-1-one
Inchi: InChI=1S/C10H16O2/c1-4-12-9-5-8(11)6-10(2,3)7-9/h5H,4,6-7H2,1-3H3
InchiKey: HALCXXAVLJHSTJ-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CCOC1=CC(=O)CC(C)(C)C1
Mol. weight [g/mol]: 168.23
CAS: 6267-39-6

Physical Properties

Property code	Value	Unit	Source
gf	-154.98	kJ/mol	Joback Method
hf	-403.78	kJ/mol	Joback Method
hfus	8.72	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
ie	8.87	eV	NIST Webbook
log10ws	-2.38		Crippen Method
logp	2.296		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
tb	542.37	K	Joback Method
tc	765.73	K	Joback Method
tf	337.47	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.46	J/mol×K	542.37	Joback Method
cpg	363.25	J/mol×K	579.60	Joback Method
cpg	379.19	J/mol×K	616.82	Joback Method
cpg	394.35	J/mol×K	654.05	Joback Method
cpg	408.82	J/mol×K	691.28	Joback Method
cpg	422.65	J/mol×K	728.51	Joback Method

cpg	435.91	J/mol×K	765.73	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=C6267396&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
ie:	Ionization energy
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