2,5-Cyclohexadien-1-one, 4-ethyl-3,4-dimethyl-

Other names: 4-ethyl-3,4-dimethyl-2,5-cyclohexadien-1-one
Inchi: InChI=1S/C10H14O/c1-4-10(3)6-5-9(11)7-8(10)2/h5-7H,4H2,1-3H3
InchiKey: CQBBARRJOASBCR-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CCC1(C)C=CC(=O)C=C1C
Mol. weight [g/mol]: 150.22
CAS: 17429-35-5

Physical Properties

Property code	Value	Unit	Source
gf	-20.02	kJ/mol	Joback Method
hf	-213.78	kJ/mol	Joback Method
hfus	8.76	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.488		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
ripol	1629.00		NIST Webbook
tb	519.11	K	Joback Method
tc	747.52	K	Joback Method
tf	316.00	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.30	J/mol×K	519.11	Joback Method
cpg	319.23	J/mol×K	557.18	Joback Method
cpg	334.23	J/mol×K	595.25	Joback Method
cpg	348.40	J/mol×K	633.31	Joback Method
cpg	361.84	J/mol×K	671.38	Joback Method
cpg	374.63	J/mol×K	709.45	Joback Method
cpg	386.88	J/mol×K	747.52	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=C17429355&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume