2,5-Cyclohexadien-1-one, 3,4,4-trimethyl-

Other names: 3,4,4-Trimethyl-2,5-cyclohexadienone
3,4,4-Trimethoxycyclohexa-2,5-dienone
Inchi: InChI=1S/C9H12O/c1-7-6-8(10)4-5-9(7,2)3/h4-6H,1-3H3
InchiKey: XWYNZKIPFPUMPJ-UHFFFAOYSA-N
Formula: C9H12O
SMILES: CC1=CC(=O)C=CC1(C)C
Mol. weight [g/mol]: 136.19
CAS: 17429-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-28.44	kJ/mol	Joback Method
hf	-193.14	kJ/mol	Joback Method
hfus	6.17	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.098		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
tb	496.23	K	Joback Method
tc	728.82	K	Joback Method
tf	304.73	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.95	J/mol×K	496.23	Joback Method
cpg	273.90	J/mol×K	535.00	Joback Method
cpg	287.94	J/mol×K	573.76	Joback Method
cpg	301.16	J/mol×K	612.53	Joback Method
cpg	313.66	J/mol×K	651.29	Joback Method

cpg	325.54	J/mol×K	690.06	Joback Method
cpg	336.88	J/mol×K	728.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C17429311&Units=SI

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