2-Cyclohexen-1-one, 4,4,6-trimethyl-

Other names: 4,4,6-Trimethyl-2-cyclohexen-1-one
4,4,6-Trimethyl-2-cyclohexenone
4,4,6-trimethylcyclohex-2-en-1-one
Inchi: InChI=1S/C9H14O/c1-7-6-9(2,3)5-4-8(7)10/h4-5,7H,6H2,1-3H3
InchiKey: PLXVUZMJQPEWPH-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1CC(C)(C)C=CC1=O
Mol. weight [g/mol]: 138.21
CAS: 13395-73-8

Physical Properties

Property code	Value	Unit	Source
gf	-56.48	kJ/mol	Joback Method
hf	-259.79	kJ/mol	Joback Method
hfus	6.41	kJ/mol	Joback Method
hvap	39.14	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.178		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
ripol	1646.00		NIST Webbook
ripol	1646.00		NIST Webbook
tb	487.42	K	Joback Method
tc	716.11	K	Joback Method
tf	287.21	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.00	J/mol×K	487.42	Joback Method
cpg	293.16	J/mol×K	525.54	Joback Method
cpg	309.30	J/mol×K	563.65	Joback Method
cpg	324.53	J/mol×K	601.77	Joback Method

cpg	338.92	J/mol×K	639.88	Joback Method
cpg	352.57	J/mol×K	678.00	Joback Method
cpg	365.56	J/mol×K	716.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13395738&Units=SI
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

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