2-Cyclopenten-1-one, 3,4,4-trimethyl-

Other names: 3,4,4-trimethyl-2-cyclopenten-1-one
Inchi: InChI=1S/C8H12O/c1-6-4-7(9)5-8(6,2)3/h4H,5H2,1-3H3
InchiKey: BDINBSUUIUWFNH-UHFFFAOYSA-N
Formula: C8H12O
SMILES: CC1=CC(=O)CC1(C)C
Mol. weight [g/mol]: 124.18
CAS: 30434-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-54.72	kJ/mol	Joback Method
hf	-224.12	kJ/mol	Joback Method
hfus	4.46	kJ/mol	Joback Method
hvap	37.71	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
rinpol	1064.00		NIST Webbook
tb	469.92	K	Joback Method
tc	695.04	K	Joback Method
tf	296.22	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.07	J/mol×K	469.92	Joback Method
cpg	247.29	J/mol×K	507.44	Joback Method
cpg	260.65	J/mol×K	544.96	Joback Method
cpg	273.23	J/mol×K	582.48	Joback Method
cpg	285.12	J/mol×K	620.00	Joback Method
cpg	296.41	J/mol×K	657.52	Joback Method
cpg	307.19	J/mol×K	695.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30434652&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

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