

2-Cyclopenten-1-one, 3,5,5-trimethyl-

Other names:	3,5,5-Trimethyl-2-cyclopenten-1-one 3,5,5-Trimethyl-2-cyclopentenone 3,5,5-Trimethyl-cyclopent-2-en-1-one
Inchi:	InChI=1S/C8H12O/c1-6-4-7(9)8(2,3)5-6/h4H,5H2,1-3H3
InchiKey:	AVXVDNJFGZNVAB-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CC1=CC(=O)C(C)(C)C1
Mol. weight [g/mol]:	124.18
CAS:	24156-95-4

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
ripol	1617.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1644.00		NIST Webbook
ripol	1617.00		NIST Webbook
tb	469.92	K	Joback Method
tc	695.04	K	Joback Method
tf	296.22	K	Joback Method
vc	0.415	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24156954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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