

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

Other names:	3,4-dimethylcyclopent-2-en-1-one
Inchi:	InChI=1S/C7H10O/c1-5-3-7(8)4-6(5)2/h3,6H,4H2,1-2H3
InchiKey:	XSOSLVVAKBKYRV-UHFFFAOYSA-N
Formula:	C7H10O
SMILES:	CC1=CC(=O)CC1C
Mol. weight [g/mol]:	110.15
CAS:	30434-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-57.65	kJ/mol	Joback Method
hf	-218.72	kJ/mol	Joback Method
hfus	8.16	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.542		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
ripol	1439.00		NIST Webbook
tb	446.80	K	Joback Method
tc	665.38	K	Joback Method
tf	261.05	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.39	J/molxK	446.80	Joback Method
cpg	204.25	J/molxK	483.23	Joback Method
cpg	216.60	J/molxK	519.66	Joback Method
cpg	228.43	J/molxK	556.09	Joback Method
cpg	239.73	J/molxK	592.52	Joback Method
cpg	250.51	J/molxK	628.95	Joback Method
cpg	260.75	J/molxK	665.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30434641&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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