

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

Other names:	2,3,4-Trimethyl-2-cyclopenten-1-one Cyclopent-2-ene-1-one, 2,3,4-trimethyl- 2,3,4-trimethylcyclopenten-1-one
Inchi:	InChI=1S/C8H12O/c1-5-4-8(9)7(3)6(5)2/h5H,4H2,1-3H3
InchiKey:	QQQNTXCURBPBOK-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CC1=C(C)C(C)CC1=O
Mol. weight [g/mol]:	124.18
CAS:	28790-86-5

Physical Properties

Property code	Value	Unit	Source
gf	-58.86	kJ/mol	Joback Method
hf	-250.83	kJ/mol	Joback Method
hfus	10.37	kJ/mol	Joback Method
hvap	39.52	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.932		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
ripol	1058.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1071.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1539.00		NIST Webbook
tb	474.66	K	Joback Method
tc	691.44	K	Joback Method
tf	284.84	K	Joback Method
vc	0.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.98	J/molxK	474.66	Joback Method
cpg	246.74	J/molxK	510.79	Joback Method
cpg	259.97	J/molxK	546.92	Joback Method
cpg	272.67	J/molxK	583.05	Joback Method
cpg	284.81	J/molxK	619.18	Joback Method
cpg	296.41	J/molxK	655.31	Joback Method
cpg	307.43	J/molxK	691.44	Joback Method

Sources

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=C28790865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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