

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

Other names:	2,3,5-Trimethyl-2-cyclopenten-1-one
Inchi:	InChI=1S/C8H12O/c1-5-4-6(2)8(9)7(5)3/h6H,4H2,1-3H3
InchiKey:	HNZWNWPTJZTRTK-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CC1=C(C)C(=O)C(C)C1
Mol. weight [g/mol]:	124.18

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	1592.00		NIST Webbook
ripol	1592.00		NIST Webbook
tb	474.66	K	Joback Method
tc	691.44	K	Joback Method
tf	284.84	K	Joback Method
vc	0.417	m3/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:	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R242210&Units=SI

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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