

2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl, cis

Other names:	cis-2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one cis-2-Cyclopenten-1-one, 2-hydroxy-3,4,5-trimethyl
Inchi:	InChI=1S/C8H12O2/c1-4-5(2)7(9)8(10)6(4)3/h4-5,10H,1-3H3/t4-,5+/m1/s1
InchiKey:	RMXYMRMUZJILGN-UHNVWZDZSA-N
Formula:	C8H12O2
SMILES:	CC1=C(O)C(=O)C(C)C1C
Mol. weight [g/mol]:	140.18

Physical Properties

Property code	Value	Unit	Source
gf	-203.39	kJ/mol	Joback Method
hf	-423.40	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.673		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
ripol	1826.00		NIST Webbook
ripol	1826.00		NIST Webbook
ripol	1826.00		NIST Webbook
tb	562.17	K	Joback Method
tc	764.08	K	Joback Method
tf	341.42	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.47	J/molxK	562.17	Joback Method
cpg	297.71	J/molxK	595.82	Joback Method
cpg	309.44	J/molxK	629.47	Joback Method

cpg	320.67	J/mol×K	663.12	Joback Method
cpg	331.38	J/mol×K	696.77	Joback Method
cpg	341.56	J/mol×K	730.42	Joback Method
cpg	351.19	J/mol×K	764.08	Joback Method

Sources

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=R53329&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/42-091-4/2-Cyclopenten-1-one-2-hydroxy-3-4-5-trimethyl-cis.pdf>

Generated by Cheméo on 2024-04-17 03:09:34.049337838 +0000 UTC m=+15612622.969915149.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.