

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

Other names:	trans-2-Hydroxy-3,4,5-trimethyl-2-cyclopenten-1-one trans-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-/m0/s1
InchiKey:	RMXYMRMUZJILGN-WHFBIAKZSA-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	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1733.00		NIST Webbook
tb	562.17	K	Joback Method
tc	764.08	K	Joback Method
tf	341.42	K	Joback Method
vc	0.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.47	J/mol×K	562.17	Joback Method
cpg	297.71	J/mol×K	595.82	Joback Method

cpg	309.44	J/mol×K	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53333&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
rinpola:	Non-polar retention indices
ripola:	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/64-970-4/2-Cyclopenten-1-one-2-hydroxy-3-4-5-trimethyl-trans.pdf>

Generated by Cheméo on 2024-04-25 17:23:55.741312939 +0000 UTC m=+16355084.661890256.

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