

2,3,5,5-Tetramethyl-4-methylene-2-cyclopenten-1-

Inchi:	InChI=1S/C9H14O/c1-6-5-9(3,4)8(10)7(6)2/h5H2,1-4H3
InchiKey:	FYDYTXLWBFWFBW-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC1=C(C)C(=O)C(C)(C)C1
Mol. weight [g/mol]:	138.21

Physical Properties

Property code	Value	Unit	Source
gf	-55.93	kJ/mol	Joback Method
hf	-256.23	kJ/mol	Joback Method
hfus	6.66	kJ/mol	Joback Method
hvap	40.60	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.322		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1171.00		NIST Webbook
rinpol	1171.00		NIST Webbook
tb	497.78	K	Joback Method
tc	720.53	K	Joback Method
tf	320.01	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.32	J/mol×K	497.78	Joback Method
cpg	291.17	J/mol×K	534.91	Joback Method
cpg	305.21	J/mol×K	572.03	Joback Method
cpg	318.53	J/mol×K	609.16	Joback Method
cpg	331.20	J/mol×K	646.28	Joback Method
cpg	343.31	J/mol×K	683.41	Joback Method
cpg	354.96	J/mol×K	720.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R342231&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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