

2,3,3-Trimethyl-2-(3-methyl-buta-1,3-dienyl)-cyclohexanone

Other names:	2,3,3-Trimethyl-2-(3-methyl-1,3-butadienyl)-cyclohexanone
Inchi:	InChI=1S/C14H22O/c1-11(2)8-10-14(5)12(15)7-6-9-13(14,3)4/h8,10H,1,6-7,9H2,2-5H3/b
InchiKey:	BUIXYBRVJFSDRY-CSKARUKUSA-N
Formula:	C14H22O
SMILES:	<chem>C=C(C)C=CC1(C)C(=O)CCCC1(C)C</chem>
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	109.68	kJ/mol	Joback Method
hf	-172.67	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	48.19	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.904		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	603.62	K	Joback Method
tc	837.90	K	Joback Method
tf	345.90	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.57	J/mol×K	603.62	Joback Method
cpg	518.43	J/mol×K	642.67	Joback Method
cpg	538.15	J/mol×K	681.71	Joback Method
cpg	556.99	J/mol×K	720.76	Joback Method
cpg	575.19	J/mol×K	759.81	Joback Method
cpg	593.00	J/mol×K	798.85	Joback Method
cpg	610.66	J/mol×K	837.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U193606&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
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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