

# 4-Methyl-1-(1,2,2-trimethylcyclopentyl)cyclohex-3

<b>Inchi:</b>	InChI=1S/C15H26O/c1-12-6-10-15(16,11-7-12)14(4)9-5-8-13(14,2)3/h6,16H,5,7-11H2,1-
<b>InchiKey:</b>	JXGLOXHHKFQUPA-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	CC1=CCC(O)(C2(C)CCCC2(C)C)CC1
<b>Mol. weight [g/mol]:</b>	222.37
<b>CAS:</b>	943525-66-4

## Physical Properties

Property code	Value	Unit	Source
gf	-4.25	kJ/mol	Joback Method
hf	-318.67	kJ/mol	Joback Method
hfus	7.47	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.064		Crippen Method
mcpvol	202.060	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1715.40		NIST Webbook
rinpol	1702.80		NIST Webbook
rinpol	1702.80		NIST Webbook
tb	669.80	K	Joback Method
tc	892.10	K	Joback Method
tf	418.65	K	Joback Method
vc	0.748	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.96	J/molxK	669.80	Joback Method
cpg	610.99	J/molxK	706.85	Joback Method
cpg	630.41	J/molxK	743.90	Joback Method
cpg	649.54	J/molxK	780.95	Joback Method
cpg	668.73	J/molxK	818.00	Joback Method
cpg	688.28	J/molxK	855.05	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C943525664&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C943525664&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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