

# cis-Methylisocosticate

<b>Inchi:</b>	InChI=1S/C16H24O2/c1-11-6-5-8-16(3)9-7-13(10-14(11)16)12(2)15(17)18-4/h13H,2,5-10
<b>InchiKey:</b>	OWZSHJKGKHTKDS-XJKSGUPXSA-N
<b>Formula:</b>	C16H24O2
<b>SMILES:</b>	C=C(C(=O)OC)C1CCC2(C)CCCC(C)=C2C1
<b>Mol. weight [g/mol]:</b>	248.36

## Physical Properties

Property code	Value	Unit	Source
gf	7.52	kJ/mol	Joback Method
hf	-331.69	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.022		Crippen Method
mvol	213.420	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	678.25	K	Joback Method
tc	903.67	K	Joback Method
tf	398.02	K	Joback Method
vc	0.803	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.26	J/mol×K	678.25	Joback Method
cpg	629.72	J/mol×K	715.82	Joback Method
cpg	649.10	J/mol×K	753.39	Joback Method
cpg	667.55	J/mol×K	790.96	Joback Method
cpg	685.22	J/mol×K	828.53	Joback Method
cpg	702.26	J/mol×K	866.10	Joback Method
cpg	718.81	J/mol×K	903.67	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R590544&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R590544&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>
<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>

# 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>rinpola:</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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