

# 6-heptadecalactone

<b>Inchi:</b>	InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-12-15-13-10-11-14-16(17)18-15/h15H,2-14H2,1
<b>InchiKey:</b>	JDBCCUBGERLOBZ-UHFFFAOYSA-N
<b>Formula:</b>	C16H30O2
<b>SMILES:</b>	CCCCCCCCCCC1CCCCC(=O)O1
<b>Mol. weight [g/mol]:</b>	254.41

## Physical Properties

Property code	Value	Unit	Source
gf	-112.52	kJ/mol	Joback Method
hf	-595.11	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	60.57	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.003		Crippen Method
mvol	232.880	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
ripol	2903.00		NIST Webbook
ripol	2903.00		NIST Webbook
tb	684.07	K	Joback Method
tc	884.29	K	Joback Method
tf	368.73	K	Joback Method
vc	0.884	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.78	J/mol×K	684.07	Joback Method
cpg	715.34	J/mol×K	717.44	Joback Method
cpg	735.70	J/mol×K	750.81	Joback Method
cpg	754.86	J/mol×K	784.18	Joback Method
cpg	772.82	J/mol×K	817.55	Joback Method
cpg	789.59	J/mol×K	850.92	Joback Method
cpg	805.19	J/mol×K	884.29	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=R320424&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R320424&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>ri pol:</b>	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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