

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, ethyl 2-ethylbutyl ester

<b>Inchi:</b>	InChI=1S/C16H26O4/c1-4-12(5-2)11-20-16(18)14-10-8-7-9-13(14)15(17)19-6-3/h7-8,12-
<b>InchiKey:</b>	UNRCMOQMXSQDKE-UHFFFAOYSA-N
<b>Formula:</b>	C16H26O4
<b>SMILES:</b>	CCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
<b>Mol. weight [g/mol]:</b>	282.38

## Physical Properties

Property code	Value	Unit	Source
gf	-339.74	kJ/mol	Joback Method
hf	-776.69	kJ/mol	Joback Method
hfus	33.37	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.111		Crippen Method
mvol	236.020	ml/mol	McGowan Method
pc	1671.43	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	731.66	K	Joback Method
tc	931.82	K	Joback Method
tf	403.30	K	Joback Method
vc	0.891	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.67	J/molxK	731.66	Joback Method
cpg	724.87	J/molxK	765.02	Joback Method
cpg	741.91	J/molxK	798.38	Joback Method
cpg	757.81	J/molxK	831.74	Joback Method
cpg	772.57	J/molxK	865.10	Joback Method
cpg	786.20	J/molxK	898.46	Joback Method
cpg	798.70	J/molxK	931.82	Joback Method
dvisc	0.0016405	Paxs	403.30	Joback Method

dvisc	0.0008124	Paxs	458.03	Joback Method
dvisc	0.0004674	Paxs	512.75	Joback Method
dvisc	0.0002992	Paxs	567.48	Joback Method
dvisc	0.0002071	Paxs	622.21	Joback Method
dvisc	0.0001522	Paxs	676.93	Joback Method
dvisc	0.0001171	Paxs	731.66	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U382804&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382804&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>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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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