

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, ethyl 3-phenylpropyl ester

Inchi:	InChI=1S/C19H24O4/c1-2-22-18(20)16-12-6-7-13-17(16)19(21)23-14-8-11-15-9-4-3-5-10
InchiKey:	IIFLFIBYMGAWNO-UHFFFAOYSA-N
Formula:	C19H24O4
SMILES:	CCOC(=O)C1CC=CCC1C(=O)OCCCc1ccccc1
Mol. weight [g/mol]:	316.39

## Physical Properties

Property code	Value	Unit	Source
gf	-199.63	kJ/mol	Joback Method
hf	-596.80	kJ/mol	Joback Method
hfus	38.71	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.308		Crippen Method
mvol	254.530	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2343.00		NIST Webbook
tb	827.42	K	Joback Method
tc	1048.85	K	Joback Method
tf	478.53	K	Joback Method
vc	0.958	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.53	J/molxK	827.42	Joback Method
cpg	807.29	J/molxK	864.32	Joback Method
cpg	822.58	J/molxK	901.23	Joback Method
cpg	836.43	J/molxK	938.13	Joback Method
cpg	848.87	J/molxK	975.04	Joback Method
cpg	859.93	J/molxK	1011.94	Joback Method
cpg	869.64	J/molxK	1048.85	Joback Method
dvisc	0.0009214	Paxs	478.53	Joback Method
dvisc	0.0005056	Paxs	536.68	Joback Method

dvisc	0.0003120	Paxs	594.83	Joback Method
dvisc	0.0002098	Paxs	652.98	Joback Method
dvisc	0.0001506	Paxs	711.12	Joback Method
dvisc	0.0001136	Paxs	769.27	Joback Method
dvisc	0.0000892	Paxs	827.42	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=U382772&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382772&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>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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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