

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

Inchi:	InChI=1S/C23H40O4/c1-4-7-8-9-10-11-14-17-26-22(24)20-15-12-13-16-21(20)23(25)27-
InchiKey:	NHPILMWQURCDSG-UHFFFAOYSA-N
Formula:	C23H40O4
SMILES:	CCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
Mol. weight [g/mol]:	380.56

## Physical Properties

Property code	Value	Unit	Source
gf	-280.80	kJ/mol	Joback Method
hf	-921.17	kJ/mol	Joback Method
hfus	51.50	kJ/mol	Joback Method
hvap	85.13	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.842		Crippen Method
mcvol	334.650	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2533.00		NIST Webbook
tb	891.82	K	Joback Method
tc	1094.61	K	Joback Method
tf	482.19	K	Joback Method
vc	1.284	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.49	J/molxK	891.82	Joback Method
cpg	1145.43	J/molxK	925.62	Joback Method
cpg	1162.89	J/molxK	959.42	Joback Method
cpg	1178.89	J/molxK	993.22	Joback Method
cpg	1193.46	J/molxK	1027.01	Joback Method
cpg	1206.62	J/molxK	1060.81	Joback Method
cpg	1218.41	J/molxK	1094.61	Joback Method
dvisc	0.0008228	Paxs	482.19	Joback Method
dvisc	0.0003773	Paxs	550.46	Joback Method

dvisc	0.0002055	Paxs	618.73	Joback Method
dvisc	0.0001263	Paxs	687.00	Joback Method
dvisc	0.0000847	Paxs	755.28	Joback Method
dvisc	0.0000608	Paxs	823.55	Joback Method
dvisc	0.0000458	Paxs	891.82	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=U382811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382811&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>

## 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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