

# cis-Cyclohex-4-en-1,2-dicarboxylic acid, 3-methylbutyl octyl ester

<b>Inchi:</b>	InChI=1S/C21H36O4/c1-4-5-6-7-8-11-15-24-20(22)18-12-9-10-13-19(18)21(23)25-16-14
<b>InchiKey:</b>	RTQFRCFDNQOMRT-UHFFFAOYSA-N
<b>Formula:</b>	C21H36O4
<b>SMILES:</b>	CCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCC(C)C
<b>Mol. weight [g/mol]:</b>	352.51

## Physical Properties

Property code	Value	Unit	Source
gf	-297.64	kJ/mol	Joback Method
hf	-879.89	kJ/mol	Joback Method
hfus	46.32	kJ/mol	Joback Method
hvap	80.68	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.062		Crippen Method
mvol	306.470	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	846.06	K	Joback Method
tc	1044.69	K	Joback Method
tf	459.65	K	Joback Method
vc	1.171	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.95	J/molxK	846.06	Joback Method
cpg	1021.70	J/molxK	879.16	Joback Method
cpg	1039.10	J/molxK	912.27	Joback Method
cpg	1055.15	J/molxK	945.37	Joback Method
cpg	1069.87	J/molxK	978.48	Joback Method
cpg	1083.30	J/molxK	1011.58	Joback Method
cpg	1095.45	J/molxK	1044.69	Joback Method
dvisc	0.0010253	Paxs	459.65	Joback Method

dvisc	0.0004795	Paxs	524.05	Joback Method
dvisc	0.0002648	Paxs	588.45	Joback Method
dvisc	0.0001644	Paxs	652.86	Joback Method
dvisc	0.0001112	Paxs	717.26	Joback Method
dvisc	0.0000802	Paxs	781.66	Joback Method
dvisc	0.0000608	Paxs	846.06	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=U382825&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382825&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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