

# 1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylphenyl ethyl ester

Inchi:	InChI=1S/C18H24O4/c1-4-21-17(19)15-7-5-6-8-16(15)18(20)22-14-10-12(2)9-13(3)11-14
InchiKey:	GCTHIAFBMYWCKT-UHFFFAOYSA-N
Formula:	C18H24O4
SMILES:	CCOC(=O)C1CCCCC1C(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	304.38

## Physical Properties

Property code	Value	Unit	Source
gf	-257.27	kJ/mol	Joback Method
hf	-656.88	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.578		Crippen Method
mvol	244.740	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
tb	815.34	K	Joback Method
tc	1039.34	K	Joback Method
tf	491.54	K	Joback Method
vc	0.915	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.78	J/molxK	815.34	Joback Method
cpg	830.71	J/molxK	1002.01	Joback Method
cpg	819.27	J/molxK	964.67	Joback Method
cpg	806.37	J/molxK	927.34	Joback Method
cpg	791.99	J/molxK	890.01	Joback Method
cpg	776.13	J/molxK	852.67	Joback Method
cpg	840.69	J/molxK	1039.34	Joback Method
dvisc	0.0000966	Paxs	815.34	Joback Method

dvisc	0.0001206	Paxs	761.37	Joback Method
dvisc	0.0001557	Paxs	707.41	Joback Method
dvisc	0.0002096	Paxs	653.44	Joback Method
dvisc	0.0002978	Paxs	599.47	Joback Method
dvisc	0.0004536	Paxs	545.51	Joback Method
dvisc	0.0007577	Paxs	491.54	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=U339611&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U339611&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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