

# Octatetraene dicarboxylic acid, dimethyl ester

<b>Inchi:</b>	InChI=1S/C12H14O4/c1-15-11(13)9-7-5-3-4-6-8-10-12(14)16-2/h3-10H,1-2H3/b5-3+,6-4-
<b>InchiKey:</b>	JZTBREXKYLZPNJ-MIIZMDLZSA-N
<b>Formula:</b>	C12H14O4
<b>SMILES:</b>	COC(=O)C=CC=CC=CC(=O)OC
<b>Mol. weight [g/mol]:</b>	222.24

## Physical Properties

Property code	Value	Unit	Source
gf	-96.80	kJ/mol	Joback Method
hf	-311.73	kJ/mol	Joback Method
hfus	33.22	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.557		Crippen Method
mcvol	177.620	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
tb	643.18	K	Joback Method
tc	847.98	K	Joback Method
tf	349.00	K	Joback Method
vc	0.675	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.73	J/molxK	643.18	Joback Method
cpg	443.15	J/molxK	677.31	Joback Method
cpg	454.85	J/molxK	711.45	Joback Method
cpg	465.86	J/molxK	745.58	Joback Method
cpg	476.24	J/molxK	779.71	Joback Method
cpg	486.04	J/molxK	813.85	Joback Method
cpg	495.29	J/molxK	847.98	Joback Method
dvisc	0.0012571	Paxs	349.00	Joback Method
dvisc	0.0006029	Paxs	398.03	Joback Method
dvisc	0.0003397	Paxs	447.06	Joback Method

dvisc	0.0002144	Paxs	496.09	Joback Method
dvisc	0.0001470	Paxs	545.12	Joback Method
dvisc	0.0001073	Paxs	594.15	Joback Method
dvisc	0.0000821	Paxs	643.18	Joback Method

## Sources

<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=B6000663&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000663&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>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/49-994-5/Octatetraene-dicarboxylic-acid-dimethyl-ester.pdf>

Generated by Cheméo on 2024-04-19 20:26:57.697594373 +0000 UTC m=+15847666.618171689.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.