

# Diethylmalonic acid, octyl 3-phenylpropyl ester

Inchi:	InChI=1S/C24H38O4/c1-4-7-8-9-10-14-19-27-22(25)24(5-2,6-3)23(26)28-20-15-18-21-16
InchiKey:	GFUVETHQOOBVIR-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	390.56

## Physical Properties

Property code	Value	Unit	Source
gf	-201.39	kJ/mol	Joback Method
hf	-800.51	kJ/mol	Joback Method
hfus	50.12	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.872		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	2594.00		NIST Webbook
tb	924.55	K	Joback Method
tc	1134.34	K	Joback Method
tf	533.40	K	Joback Method
vc	1.308	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.14	J/molxK	924.55	Joback Method
cpg	1193.58	J/molxK	1099.37	Joback Method
cpg	1181.20	J/molxK	1064.41	Joback Method
cpg	1167.73	J/molxK	1029.44	Joback Method
cpg	1153.10	J/molxK	994.48	Joback Method
cpg	1137.26	J/molxK	959.51	Joback Method
cpg	1204.94	J/molxK	1134.34	Joback Method
dvisc	0.0000232	Paxs	924.55	Joback Method
dvisc	0.0000312	Paxs	859.36	Joback Method

dvisc	0.0000439	Paxs	794.17	Joback Method
dvisc	0.0000657	Paxs	728.97	Joback Method
dvisc	0.0001064	Paxs	663.78	Joback Method
dvisc	0.0001915	Paxs	598.59	Joback Method
dvisc	0.0003979	Paxs	533.40	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=U369658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369658&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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