

# Diethylmalonic acid, 3,7-dimethyloctyl pentyl ester

Inchi:	InChI=1S/C22H42O4/c1-7-10-11-16-25-20(23)22(8-2,9-3)21(24)26-17-15-19(6)14-12-13
InchiKey:	AKMUKLMHSUODTL-UHFFFAOYSA-N
Formula:	C22H42O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]:	370.57

## Physical Properties

Property code	Value	Unit	Source
gf	-335.52	kJ/mol	Joback Method
hf	-1006.32	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	80.81	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.922		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinsol	2142.00		NIST Webbook
tb	851.23	K	Joback Method
tc	1044.28	K	Joback Method
tf	454.44	K	Joback Method
vc	1.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.48	J/molxK	851.23	Joback Method
cpg	1177.25	J/molxK	1012.11	Joback Method
cpg	1162.73	J/molxK	979.93	Joback Method
cpg	1147.14	J/molxK	947.76	Joback Method
cpg	1130.42	J/molxK	915.58	Joback Method
cpg	1112.55	J/molxK	883.41	Joback Method
cpg	1190.72	J/molxK	1044.28	Joback Method
dvisc	0.0000263	Paxs	851.23	Joback Method
dvisc	0.0000369	Paxs	785.10	Joback Method

dvisc	0.0000552	Paxs	718.97	Joback Method
dvisc	0.0000896	Paxs	652.84	Joback Method
dvisc	0.0001622	Paxs	586.70	Joback Method
dvisc	0.0003412	Paxs	520.57	Joback Method
dvisc	0.0008913	Paxs	454.44	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=U369405&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369405&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>mccvol:</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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