

# Diethylmalonic acid, di(hept-4-yl) ester

<b>Inchi:</b>	InChI=1S/C21H40O4/c1-7-13-17(14-8-2)24-19(22)21(11-5,12-6)20(23)25-18(15-9-3)16-1
<b>InchiKey:</b>	UCVAAUPRJHJSSC-UHFFFAOYSA-N
<b>Formula:</b>	C21H40O4
<b>SMILES:</b>	CCCC(CCC)OC(=O)C(CC)(CC)C(=O)OC(CCC)CCC
<b>Mol. weight [g/mol]:</b>	356.54

## Physical Properties

Property code	Value	Unit	Source
gf	-343.94	kJ/mol	Joback Method
hf	-985.68	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.817		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	828.35	K	Joback Method
tc	1018.59	K	Joback Method
tf	443.17	K	Joback Method
vc	1.236	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.95	J/molxK	828.35	Joback Method
cpg	1050.71	J/molxK	860.06	Joback Method
cpg	1068.32	J/molxK	891.76	Joback Method
cpg	1084.83	J/molxK	923.47	Joback Method
cpg	1100.26	J/molxK	955.18	Joback Method
cpg	1114.66	J/molxK	986.89	Joback Method
cpg	1128.05	J/molxK	1018.59	Joback Method
dvisc	0.0010254	Paxs	443.17	Joback Method

dvisc	0.0003951	Paxs	507.37	Joback Method
dvisc	0.0001886	Paxs	571.56	Joback Method
dvisc	0.0001045	Paxs	635.76	Joback Method
dvisc	0.0000646	Paxs	699.96	Joback Method
dvisc	0.0000432	Paxs	764.15	Joback Method
dvisc	0.0000308	Paxs	828.35	Joback Method

## Sources

<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>
<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=U370521&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370521&amp;Units=SI</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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