

# Diethylmalonic acid, 2-ethylbutyl heptyl ester

<b>Inchi:</b>	InChI=1S/C20H38O4/c1-6-11-12-13-14-15-23-18(21)20(9-4,10-5)19(22)24-16-17(7-2)8-3
<b>InchiKey:</b>	MICTWKZIWJZACN-UHFFFAOYSA-N
<b>Formula:</b>	C20H38O4
<b>SMILES:</b>	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(CC)CC
<b>Mol. weight [g/mol]:</b>	342.51

## Physical Properties

Property code	Value	Unit	Source
gf	-349.92	kJ/mol	Joback Method
hf	-959.76	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	76.74	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.286		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinsol	2007.00		NIST Webbook
tb	805.91	K	Joback Method
tc	992.86	K	Joback Method
tf	446.90	K	Joback Method
vc	1.187	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.67	J/molxK	805.91	Joback Method
cpg	989.01	J/molxK	837.07	Joback Method
cpg	1006.28	J/molxK	868.23	Joback Method
cpg	1022.51	J/molxK	899.38	Joback Method
cpg	1037.73	J/molxK	930.54	Joback Method
cpg	1051.98	J/molxK	961.70	Joback Method
cpg	1065.27	J/molxK	992.86	Joback Method
dvisc	0.0009605	Paxs	446.90	Joback Method
dvisc	0.0004114	Paxs	506.73	Joback Method

dvisc	0.0002108	Paxs	566.57	Joback Method
dvisc	0.0001227	Paxs	626.40	Joback Method
dvisc	0.0000785	Paxs	686.24	Joback Method
dvisc	0.0000540	Paxs	746.08	Joback Method
dvisc	0.0000392	Paxs	805.91	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=U370479&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370479&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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