

# Dimethylmalonic acid, isobutyl tridecyl ester

<b>Inchi:</b>	InChI=1S/C22H42O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-25-20(23)22(4,5)21(24)26-18
<b>InchiKey:</b>	NQZLLZANOKSBHI-UHFFFAOYSA-N
<b>Formula:</b>	C22H42O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	370.57

## Physical Properties

Property code	Value	Unit	Source
gf	-333.08	kJ/mol	Joback Method
hf	-1001.04	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.066		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2299.00		NIST Webbook
tb	851.67	K	Joback Method
tc	1044.13	K	Joback Method
tf	469.44	K	Joback Method
vc	1.298	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/molxK	851.67	Joback Method
cpg	1112.04	J/molxK	883.75	Joback Method
cpg	1129.88	J/molxK	915.82	Joback Method
cpg	1146.58	J/molxK	947.90	Joback Method
cpg	1162.18	J/molxK	979.97	Joback Method
cpg	1176.71	J/molxK	1012.05	Joback Method
cpg	1190.22	J/molxK	1044.13	Joback Method
dvisc	0.0007385	Paxs	469.44	Joback Method
dvisc	0.0003111	Paxs	533.14	Joback Method

dvisc	0.0001576	Paxs	596.85	Joback Method
dvisc	0.0000910	Paxs	660.56	Joback Method
dvisc	0.0000579	Paxs	724.26	Joback Method
dvisc	0.0000396	Paxs	787.97	Joback Method
dvisc	0.0000287	Paxs	851.67	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U361661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361661&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>
<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>

## 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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