

# Dimethylmalonic acid, nonyl 2,2,3,3,3-pentafluoropropyl ester

<b>Inchi:</b>	InChI=1S/C17H27F5O4/c1-4-5-6-7-8-9-10-11-25-13(23)15(2,3)14(24)26-12-16(18,19)17
<b>InchiKey:</b>	KKWORTPTMULOCR-UHFFFAOYSA-N
<b>Formula:</b>	C17H27F5O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	390.39

## Physical Properties

Property code	Value	Unit	Source
gf	-1341.11	kJ/mol	Joback Method
hf	-1890.61	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.047		Crippen Method
mvol	274.120	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	727.60	K	Joback Method
tc	898.72	K	Joback Method
tf	435.88	K	Joback Method
vc	1.093	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.25	J/mol×K	727.60	Joback Method
cpg	850.70	J/mol×K	756.12	Joback Method
cpg	865.27	J/mol×K	784.64	Joback Method
cpg	878.99	J/mol×K	813.16	Joback Method
cpg	891.92	J/mol×K	841.68	Joback Method
cpg	904.10	J/mol×K	870.20	Joback Method
cpg	915.56	J/mol×K	898.72	Joback Method

# Sources

<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=U361943&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361943&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>rinpola:</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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