

# Dimethylmalonic acid, heptadecyl 2,2,3,3-tetrafluoropropyl ester

Inchi:	InChI=1S/C25H44F4O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-32-22(30)24(2,3
InchiKey:	QOOSCMSYKYZANB-UHFFFAOYSA-N
Formula:	C25H44F4O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	484.61

## Physical Properties

Property code	Value	Unit	Source
gf	-1084.22	kJ/mol	Joback Method
hf	-1856.15	kJ/mol	Joback Method
hfus	60.05	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-8.40		Crippen Method
logp	7.871		Crippen Method
mcvol	385.070	ml/mol	McGowan Method
pc	746.51	kPa	Joback Method
rinsol	2501.00		NIST Webbook
tb	914.16	K	Joback Method
tc	1124.99	K	Joback Method
tf	508.03	K	Joback Method
vc	1.528	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1309.34	J/molxK	914.16	Joback Method
cpg	1329.39	J/molxK	949.30	Joback Method
cpg	1348.06	J/molxK	984.44	Joback Method
cpg	1365.41	J/molxK	1019.57	Joback Method
cpg	1381.53	J/molxK	1054.71	Joback Method
cpg	1396.51	J/molxK	1089.85	Joback Method
cpg	1410.43	J/molxK	1124.99	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=U361927&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361927&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvac:</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>mccol:</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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