

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

<b>Inchi:</b>	InChI=1S/C14H21F5O4/c1-9(2)6-5-7-22-10(20)12(3,4)11(21)23-8-13(15,16)14(17,18)19
<b>InchiKey:</b>	HWDZIZYJDBYSPA-UHFFFAOYSA-N
<b>Formula:</b>	C14H21F5O4
<b>SMILES:</b>	CC(C)CCCOC(=O)C(C)(C)C(=O)OCC(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	348.31

## Physical Properties

Property code	Value	Unit	Source
gf	-1368.81	kJ/mol	Joback Method
hf	-1833.97	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.733		Crippen Method
mvol	231.850	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
tb	658.52	K	Joback Method
tc	828.71	K	Joback Method
tf	387.07	K	Joback Method
vc	0.918	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.23	J/molxK	658.52	Joback Method
cpg	684.69	J/molxK	686.88	Joback Method
cpg	698.32	J/molxK	715.25	Joback Method
cpg	711.14	J/molxK	743.61	Joback Method
cpg	723.21	J/molxK	771.98	Joback Method
cpg	734.54	J/molxK	800.34	Joback Method
cpg	745.19	J/molxK	828.71	Joback Method

# Sources

<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=U361939&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U361939&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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