

# Malonic acid, hexyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi:	InChI=1S/C14H18F8O4/c1-2-3-4-5-6-25-9(23)7-10(24)26-8-12(17,18)14(21,22)13(19,20)
InchiKey:	NSLKIXCEBZTNBG-UHFFFAOYSA-N
Formula:	C14H18F8O4
SMILES:	CCCCCOC(=O)CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]:	402.28

## Physical Properties

Property code	Value	Unit	Source
gf	-1953.24	kJ/mol	Joback Method
hf	-2422.30	kJ/mol	Joback Method
hfus	36.46	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.214		Crippen Method
mvol	237.160	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	656.33	K	Joback Method
tc	813.73	K	Joback Method
tf	388.84	K	Joback Method
vc	0.973	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.10	J/molxK	656.33	Joback Method
cpg	707.36	J/molxK	682.56	Joback Method
cpg	719.88	J/molxK	708.80	Joback Method
cpg	731.69	J/molxK	735.03	Joback Method
cpg	742.81	J/molxK	761.27	Joback Method
cpg	753.29	J/molxK	787.50	Joback Method
cpg	763.16	J/molxK	813.73	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=U349350&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U349350&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>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>mccvol:</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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