

# Sebacic acid, isohexyl pentafluorophenyl ester

<b>Inchi:</b>	InChI=1S/C22H29F5O4/c1-14(2)10-9-13-30-15(28)11-7-5-3-4-6-8-12-16(29)31-22-20(26)
<b>InchiKey:</b>	QGXFVBAGVGANKE-UHFFFAOYSA-N
<b>Formula:</b>	C22H29F5O4
<b>SMILES:</b>	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	452.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1245.71	kJ/mol	Joback Method
hf	-1793.66	kJ/mol	Joback Method
hfus	62.28	kJ/mol	Joback Method
hvap	83.99	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.388		Crippen Method
mvol	320.810	ml/mol	McGowan Method
pc	977.17	kPa	Joback Method
rmpol	2447.00		NIST Webbook
tb	902.83	K	Joback Method
tc	1105.91	K	Joback Method
tf	558.99	K	Joback Method
vc	1.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.95	J/molxK	902.83	Joback Method
cpg	1046.26	J/molxK	936.68	Joback Method
cpg	1060.31	J/molxK	970.52	Joback Method
cpg	1073.11	J/molxK	1004.37	Joback Method
cpg	1084.68	J/molxK	1038.22	Joback Method
cpg	1095.02	J/molxK	1072.06	Joback Method
cpg	1104.14	J/molxK	1105.91	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=U355027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355027&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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