

# Sebacic acid, octyl pentafluorophenyl ester

**Inchi:** InChI=1S/C24H33F5O4/c1-2-3-4-5-10-13-16-32-17(30)14-11-8-6-7-9-12-15-18(31)33-24  
**InchiKey:** ONZXEDCRYFOGBX-UHFFFAOYSA-N  
**Formula:** C24H33F5O4  
**SMILES:** CCCCCCOC(=O)CCCCCCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 480.51

## Physical Properties

Property code	Value	Unit	Source
gf	-1226.43	kJ/mol	Joback Method
hf	-1829.66	kJ/mol	Joback Method
hfus	70.99	kJ/mol	Joback Method
hvap	88.83	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.312		Crippen Method
mvol	348.990	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2674.00		NIST Webbook
rinpol	2674.00		NIST Webbook
tb	949.03	K	Joback Method
tc	1168.11	K	Joback Method
tf	596.53	K	Joback Method
vc	1.409	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.76	J/mol×K	949.03	Joback Method
cpg	1168.12	J/mol×K	985.54	Joback Method
cpg	1182.95	J/mol×K	1022.06	Joback Method
cpg	1196.26	J/mol×K	1058.57	Joback Method
cpg	1208.08	J/mol×K	1095.08	Joback Method
cpg	1218.42	J/mol×K	1131.60	Joback Method
cpg	1227.32	J/mol×K	1168.11	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=U355030&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355030&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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