

# Sebacic acid, butyl 2-(pentafluorophenoxy)ethyl ester

Inchi:	InChI=1S/C22H29F5O5/c1-2-3-12-30-15(28)10-8-6-4-5-7-9-11-16(29)31-13-14-32-22-20
InchiKey:	VQMORFDMMGKYES-UHFFFAOYSA-N
Formula:	C22H29F5O5
SMILES:	CCCCOC(=O)CCCCCCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	468.45

## Physical Properties

Property code	Value	Unit	Source
gf	-1348.27	kJ/mol	Joback Method
hf	-1920.60	kJ/mol	Joback Method
hfus	66.99	kJ/mol	Joback Method
hvap	86.79	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.768		Crippen Method
mcvol	326.680	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	2505.00		NIST Webbook
rinpol	2505.00		NIST Webbook
tb	925.69	K	Joback Method
tc	1136.12	K	Joback Method
tf	596.22	K	Joback Method
vc	1.315	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.42	J/molxK	925.69	Joback Method
cpg	1074.42	J/molxK	960.76	Joback Method
cpg	1087.98	J/molxK	995.83	Joback Method
cpg	1100.09	J/molxK	1030.91	Joback Method
cpg	1110.74	J/molxK	1065.98	Joback Method
cpg	1119.95	J/molxK	1101.05	Joback Method
cpg	1127.70	J/molxK	1136.12	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=U416782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416782&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>

# 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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