

# Fumaric acid, dodecyl pentafluorophenyl ester

**Inchi:** InChI=1S/C22H27F5O4/c1-2-3-4-5-6-7-8-9-10-11-14-30-15(28)12-13-16(29)31-22-20(26)  
**InchiKey:** QJOUEYYAXHWNKI-OUKQBFOZSA-N  
**Formula:** C22H27F5O4  
**SMILES:** CCCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F  
**Mol. weight [g/mol]:** 450.44

## Physical Properties

Property code	Value	Unit	Source
gf	-1163.05	kJ/mol	Joback Method
hf	-1671.16	kJ/mol	Joback Method
hfus	66.01	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.308		Crippen Method
mvol	316.510	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	907.43	K	Joback Method
tc	1111.31	K	Joback Method
tf	568.91	K	Joback Method
vc	1.278	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.81	J/molxK	907.43	Joback Method
cpg	1017.59	J/molxK	941.41	Joback Method
cpg	1031.23	J/molxK	975.39	Joback Method
cpg	1043.75	J/molxK	1009.37	Joback Method
cpg	1055.18	J/molxK	1043.35	Joback Method
cpg	1065.53	J/molxK	1077.33	Joback Method
cpg	1074.83	J/molxK	1111.31	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348104&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348104&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvpap:</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>rinppl:</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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