

# Fumaric acid, nonyl pentafluorophenyl ester

<b>Inchi:</b>	InChI=1S/C19H21F5O4/c1-2-3-4-5-6-7-8-11-27-12(25)9-10-13(26)28-19-17(23)15(21)14
<b>InchiKey:</b>	TXNAWYNXEJXVAW-MDZDMXLPSA-N
<b>Formula:</b>	C19H21F5O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	408.36

## Physical Properties

Property code	Value	Unit	Source
gf	-1188.31	kJ/mol	Joback Method
hf	-1609.24	kJ/mol	Joback Method
hfus	58.24	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.138		Crippen Method
mcvol	274.240	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpola	2140.00		NIST Webbook
rinpola	2140.00		NIST Webbook
tb	838.79	K	Joback Method
tc	1028.98	K	Joback Method
tf	535.10	K	Joback Method
vc	1.109	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.79	J/mol×K	838.79	Joback Method
cpg	840.16	J/mol×K	870.49	Joback Method
cpg	852.65	J/mol×K	902.19	Joback Method
cpg	864.24	J/mol×K	933.89	Joback Method
cpg	874.97	J/mol×K	965.58	Joback Method
cpg	884.83	J/mol×K	997.28	Joback Method
cpg	893.85	J/mol×K	1028.98	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=U348101&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348101&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>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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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