

# Sebacic acid, 3-fluorophenyl nonyl ester

**Inchi:** InChI=1S/C25H39FO4/c1-2-3-4-5-8-11-14-20-29-24(27)18-12-9-6-7-10-13-19-25(28)30-2  
**InchiKey:** CURFOXKGPACISK-UHFFFAOYSA-N  
**Formula:** C25H39FO4  
**SMILES:** CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(F)c1  
**Mol. weight [g/mol]:** 422.57

## Physical Properties

Property code	Value	Unit	Source
gf	-400.25	kJ/mol	Joback Method
hf	-1019.98	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	91.68	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.146		Crippen Method
mvol	356.000	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	2988.00		NIST Webbook
rinpol	2988.00		NIST Webbook
tb	954.91	K	Joback Method
tc	1169.45	K	Joback Method
tf	555.36	K	Joback Method
vc	1.393	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.22	J/mol×K	954.91	Joback Method
cpg	1205.40	J/mol×K	990.67	Joback Method
cpg	1221.13	J/mol×K	1026.42	Joback Method
cpg	1235.46	J/mol×K	1062.18	Joback Method
cpg	1248.43	J/mol×K	1097.94	Joback Method
cpg	1260.08	J/mol×K	1133.69	Joback Method
cpg	1270.46	J/mol×K	1169.45	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=U355015&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355015&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>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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