

# Sebacic acid, 2-fluorophenyl octyl ester

<b>Inchi:</b>	InChI=1S/C24H37FO4/c1-2-3-4-5-10-15-20-28-23(26)18-11-8-6-7-9-12-19-24(27)29-22-
<b>InchiKey:</b>	QUCBTWKNRXVLLB-UHFFFAOYSA-N
<b>Formula:</b>	C24H37FO4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccccc1F
<b>Mol. weight [g/mol]:</b>	408.55

## Physical Properties

Property code	Value	Unit	Source
gf	-408.67	kJ/mol	Joback Method
hf	-999.34	kJ/mol	Joback Method
hfus	60.22	kJ/mol	Joback Method
hvap	89.45	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.756		Crippen Method
mvol	341.910	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	2903.00		NIST Webbook
tb	932.03	K	Joback Method
tc	1141.08	K	Joback Method
tf	544.09	K	Joback Method
vc	1.337	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.42	J/molxK	932.03	Joback Method
cpg	1143.28	J/molxK	966.87	Joback Method
cpg	1158.79	J/molxK	1001.71	Joback Method
cpg	1172.97	J/molxK	1036.55	Joback Method
cpg	1185.87	J/molxK	1071.39	Joback Method
cpg	1197.53	J/molxK	1106.24	Joback Method
cpg	1207.99	J/molxK	1141.08	Joback Method

# Sources

<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>
<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=U355002&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355002&amp;Units=SI</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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