

# Sebacic acid, ethyl 2-(2-fluorophenyl)ethyl ester

Inchi:	InChI=1S/C20H29FO4/c1-2-24-19(22)13-7-5-3-4-6-8-14-20(23)25-16-15-17-11-9-10-12-
InchiKey:	QDROTWXMIXINCHK-UHFFFAOYSA-N
Formula:	C20H29FO4
SMILES:	CCOC(=O)CCCCCCCC(=O)OCCc1ccccc1F
Mol. weight [g/mol]:	352.44

## Physical Properties

Property code	Value	Unit	Source
gf	-442.35	kJ/mol	Joback Method
hf	-916.78	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.595		Crippen Method
mvol	285.550	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	840.51	K	Joback Method
tc	1036.82	K	Joback Method
tf	499.01	K	Joback Method
vc	1.113	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.09	J/mol×K	840.51	Joback Method
cpg	900.82	J/mol×K	873.23	Joback Method
cpg	915.47	J/mol×K	905.95	Joback Method
cpg	929.04	J/mol×K	938.67	Joback Method
cpg	941.57	J/mol×K	971.38	Joback Method
cpg	953.08	J/mol×K	1004.10	Joback Method
cpg	963.58	J/mol×K	1036.82	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380742&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380742&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>hvp:</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>rinp:</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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