

# Sebacic acid, 2,5-difluorobenzyl heptyl ester

<b>Inchi:</b>	InChI=1S/C24H36F2O4/c1-2-3-4-9-12-17-29-23(27)13-10-7-5-6-8-11-14-24(28)30-19-20
<b>InchiKey:</b>	SWMDNXGPBIUTOU-UHFFFAOYSA-N
<b>Formula:</b>	C24H36F2O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCCCCC(=O)OCc1cc(F)ccc1F
<b>Mol. weight [g/mol]:</b>	426.54

## Physical Properties

Property code	Value	Unit	Source
gf	-613.11	kJ/mol	Joback Method
hf	-1206.92	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.642		Crippen Method
mvol	343.680	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	2828.00		NIST Webbook
rinpol	2828.00		NIST Webbook
tb	936.28	K	Joback Method
tc	1146.56	K	Joback Method
tf	557.20	K	Joback Method
vc	1.355	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.84	J/molxK	936.28	Joback Method
cpg	1149.49	J/molxK	971.33	Joback Method
cpg	1164.76	J/molxK	1006.37	Joback Method
cpg	1178.68	J/molxK	1041.42	Joback Method
cpg	1191.29	J/molxK	1076.47	Joback Method
cpg	1202.62	J/molxK	1111.51	Joback Method
cpg	1212.71	J/molxK	1146.56	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=U380766&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380766&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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