

# Succinic acid, 2,5-difluorobenzyl heptyl ester

**Inchi:** InChI=1S/C18H24F2O4/c1-2-3-4-5-6-11-23-17(21)9-10-18(22)24-13-14-12-15(19)7-8-16  
**InchiKey:** GEXJECBJEVC AKR-UHFFFAOYSA-N  
**Formula:** C18H24F2O4  
**SMILES:** CCCCCCOC(=O)CCC(=O)OCc1cc(F)ccc1F  
**Mol. weight [g/mol]:** 342.38

## Physical Properties

Property code	Value	Unit	Source
gf	-663.63	kJ/mol	Joback Method
hf	-1083.08	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	75.94	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.302		Crippen Method
mvol	259.140	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook
tb	799.00	K	Joback Method
tc	990.08	K	Joback Method
tf	489.58	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.61	J/mol×K	799.00	Joback Method
cpg	790.29	J/mol×K	830.85	Joback Method
cpg	804.01	J/mol×K	862.69	Joback Method
cpg	816.79	J/mol×K	894.54	Joback Method
cpg	828.64	J/mol×K	926.39	Joback Method
cpg	839.57	J/mol×K	958.23	Joback Method
cpg	849.60	J/mol×K	990.08	Joback Method

# Sources

<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=U381223&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381223&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>

# 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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