

# Succinic acid, 2-chloro-6-fluorobenzyl 2-methylhex-3-yl ester

<b>Inchi:</b>	InChI=1S/C18H24ClFO4/c1-4-6-16(12(2)3)24-18(22)10-9-17(21)23-11-13-14(19)7-5-8-1
<b>InchiKey:</b>	MHCJLKXWAVDYBA-UHFFFAOYSA-N
<b>Formula:</b>	C18H24ClFO4
<b>SMILES:</b>	CCCC(OC(=O)CCC(=O)OCc1c(F)cccc1Cl)C(C)C
<b>Mol. weight [g/mol]:</b>	358.83

## Physical Properties

Property code	Value	Unit	Source
gf	-485.63	kJ/mol	Joback Method
hf	-913.27	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	80.37	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.670		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	836.28	K	Joback Method
tc	1040.45	K	Joback Method
tf	488.91	K	Joback Method
vc	1.038	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.98	J/mol×K	836.28	Joback Method
cpg	810.25	J/mol×K	870.31	Joback Method
cpg	823.43	J/mol×K	904.34	Joback Method
cpg	835.54	J/mol×K	938.37	Joback Method
cpg	846.60	J/mol×K	972.40	Joback Method
cpg	856.63	J/mol×K	1006.42	Joback Method
cpg	865.63	J/mol×K	1040.45	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U380862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380862&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>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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