

# Succinic acid, 4-fluoro-3-nitrobenzyl hexyl ester

<b>Inchi:</b>	InChI=1S/C17H22FNO6/c1-2-3-4-5-10-24-16(20)8-9-17(21)25-12-13-6-7-14(18)15(11-13
<b>InchiKey:</b>	AJFLVQOKKVCAX-UHFFFAOYSA-N
<b>Formula:</b>	C17H22FNO6
<b>SMILES:</b>	CCCCCOC(=O)CCC(=O)OCc1ccc(F)c([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	355.36

## Physical Properties

Property code	Value	Unit	Source
gf	-441.69	kJ/mol	Joback Method
hf	-877.09	kJ/mol	Joback Method
hfus	53.06	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.681		Crippen Method
mvol	260.700	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	928.69	K	Joback Method
tc	1147.20	K	Joback Method
tf	621.33	K	Joback Method
vc	1.028	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.15	J/mol×K	928.69	Joback Method
cpg	829.93	J/mol×K	965.11	Joback Method
cpg	840.53	J/mol×K	1001.53	Joback Method
cpg	849.96	J/mol×K	1037.94	Joback Method
cpg	858.24	J/mol×K	1074.36	Joback Method
cpg	865.39	J/mol×K	1110.78	Joback Method
cpg	871.44	J/mol×K	1147.20	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U381021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U381021&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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