

# Glutaric acid, 3,5-difluorophenyl heptyl ester

<b>Inchi:</b>	InChI=1S/C18H24F2O4/c1-2-3-4-5-6-10-23-17(21)8-7-9-18(22)24-16-12-14(19)11-15(20)
<b>InchiKey:</b>	WZHGQUUGRVSTPG-UHFFFAOYSA-N
<b>Formula:</b>	C18H24F2O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
<b>Mol. weight [g/mol]:</b>	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	-5.50		Crippen Method
logp	4.554		Crippen Method
mcvol	259.140	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	799.00	K	Joback Method
tc	990.08	K	Joback Method
tf	489.58	K	Joback Method
vc	1.020	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.61	J/molxK	799.00	Joback Method
cpg	790.29	J/molxK	830.85	Joback Method
cpg	804.01	J/molxK	862.69	Joback Method
cpg	816.79	J/molxK	894.54	Joback Method
cpg	828.64	J/molxK	926.39	Joback Method
cpg	839.57	J/molxK	958.23	Joback Method
cpg	849.60	J/molxK	990.08	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=U358632&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358632&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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