

# Glutaric acid, 3,5-difluorophenyl octyl ester

<b>Inchi:</b>	InChI=1S/C19H26F2O4/c1-2-3-4-5-6-7-11-24-18(22)9-8-10-19(23)25-17-13-15(20)12-16
<b>InchiKey:</b>	FJIRZQKASDSNKK-UHFFFAOYSA-N
<b>Formula:</b>	C19H26F2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
<b>Mol. weight [g/mol]:</b>	356.40

## Physical Properties

Property code	Value	Unit	Source
gf	-655.21	kJ/mol	Joback Method
hf	-1103.72	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.944		Crippen Method
mvol	273.230	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	821.88	K	Joback Method
tc	1014.18	K	Joback Method
tf	500.85	K	Joback Method
vc	1.075	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.28	J/mol×K	821.88	Joback Method
cpg	848.29	J/mol×K	853.93	Joback Method
cpg	862.28	J/mol×K	885.98	Joback Method
cpg	875.29	J/mol×K	918.03	Joback Method
cpg	887.31	J/mol×K	950.08	Joback Method
cpg	898.37	J/mol×K	982.13	Joback Method
cpg	908.49	J/mol×K	1014.18	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=U358633&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358633&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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