

# Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2,3-dimethylphenyl ester

<b>Inchi:</b>	InChI=1S/C18H18F8O4/c1-10-5-3-6-12(11(10)2)30-14(28)8-4-7-13(27)29-9-16(21,22)18
<b>InchiKey:</b>	VMQPBOKBZGYPPN-UHFFFAOYSA-N
<b>Formula:</b>	C18H18F8O4
<b>SMILES:</b>	<chem>Cc1cccc(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)c1C</chem>
<b>Mol. weight [g/mol]:</b>	450.32

## Physical Properties

Property code	Value	Unit	Source
gf	-1826.41	kJ/mol	Joback Method
hf	-2291.27	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.093		Crippen Method
mcvol	269.760	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	784.49	K	Joback Method
tc	967.33	K	Joback Method
tf	485.38	K	Joback Method
vc	1.089	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/molxK	784.49	Joback Method
cpg	839.50	J/molxK	814.96	Joback Method
cpg	851.40	J/molxK	845.44	Joback Method
cpg	862.47	J/molxK	875.91	Joback Method
cpg	872.74	J/molxK	906.38	Joback Method
cpg	882.27	J/molxK	936.86	Joback Method
cpg	891.12	J/molxK	967.33	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392213&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392213&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.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>

# 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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