

# Glutaric acid, 2,5-difluorobenzyl octyl ester

<b>Inchi:</b>	InChI=1S/C20H28F2O4/c1-2-3-4-5-6-7-13-25-19(23)9-8-10-20(24)26-15-16-14-17(21)11
<b>InchiKey:</b>	VLFKABDXEFXMIG-UHFFFAOYSA-N
<b>Formula:</b>	C20H28F2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1F
<b>Mol. weight [g/mol]:</b>	370.43

## Physical Properties

Property code	Value	Unit	Source
gf	-646.79	kJ/mol	Joback Method
hf	-1124.36	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.082		Crippen Method
mvol	287.320	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rmpol	2445.00		NIST Webbook
rmpol	2445.00		NIST Webbook
tb	844.76	K	Joback Method
tc	1038.99	K	Joback Method
tf	512.12	K	Joback Method
vc	1.131	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.79	J/mol×K	844.76	Joback Method
cpg	907.11	J/mol×K	877.13	Joback Method
cpg	921.37	J/mol×K	909.50	Joback Method
cpg	934.58	J/mol×K	941.87	Joback Method
cpg	946.76	J/mol×K	974.24	Joback Method
cpg	957.92	J/mol×K	1006.62	Joback Method
cpg	968.09	J/mol×K	1038.99	Joback Method

# Sources

<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=U376950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376950&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rlnpol:</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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