

# Glutaric acid, di(4-fluorobenzyl) ester

<b>Inchi:</b>	InChI=1S/C19H18F2O4/c20-16-8-4-14(5-9-16)12-24-18(22)2-1-3-19(23)25-13-15-6-10-1
<b>InchiKey:</b>	UVFQEIFQQNGJFQ-UHFFFAOYSA-N
<b>Formula:</b>	C19H18F2O4
<b>SMILES:</b>	O=C(CCCC(=O)OCc1ccc(F)cc1)OCc1ccc(F)cc1
<b>Mol. weight [g/mol]:</b>	348.34

## Physical Properties

Property code	Value	Unit	Source
gf	-542.80	kJ/mol	Joback Method
hf	-867.19	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.922		Crippen Method
mvol	249.470	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	848.56	K	Joback Method
tc	1062.01	K	Joback Method
tf	527.27	K	Joback Method
vc	0.968	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.08	J/mol×K	848.56	Joback Method
cpg	751.06	J/mol×K	884.14	Joback Method
cpg	762.90	J/mol×K	919.71	Joback Method
cpg	773.64	J/mol×K	955.29	Joback Method
cpg	783.29	J/mol×K	990.86	Joback Method
cpg	791.90	J/mol×K	1026.44	Joback Method
cpg	799.48	J/mol×K	1062.01	Joback Method

# Sources

<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=U377486&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377486&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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