

# Glutaric acid, 2-chloro-6-fluorophenyl 2-octyl ester

Inchi:	InChI=1S/C19H26ClFO4/c1-3-4-5-6-9-14(2)24-17(22)12-8-13-18(23)25-19-15(20)10-7-1
InchiKey:	RFZZAXALYNIGNU-UHFFFAOYSA-N
Formula:	C19H26ClFO4
SMILES:	CCCCCCC(C)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	372.86

## Physical Properties

Property code	Value	Unit	Source
gf	-474.77	kJ/mol	Joback Method
hf	-928.63	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	82.98	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.457		Crippen Method
mvol	283.700	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rmpol	2423.00		NIST Webbook
rmpol	2423.00		NIST Webbook
tb	859.60	K	Joback Method
tc	1062.46	K	Joback Method
tf	515.18	K	Joback Method
vc	1.101	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.27	J/mol×K	859.60	Joback Method
cpg	867.65	J/mol×K	893.41	Joback Method
cpg	880.93	J/mol×K	927.22	Joback Method
cpg	893.13	J/mol×K	961.03	Joback Method
cpg	904.26	J/mol×K	994.84	Joback Method
cpg	914.35	J/mol×K	1028.65	Joback Method
cpg	923.41	J/mol×K	1062.46	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=U391452&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391452&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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