

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

Inchi:	InChI=1S/C17H22ClFO4/c1-2-3-4-5-12-22-15(20)10-7-11-16(21)23-17-13(18)8-6-9-14(19)
InchiKey:	YDRRKXAGOQPLMQ-UHFFFAOYSA-N
Formula:	C17H22ClFO4
SMILES:	CCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	344.81

## Physical Properties

Property code	Value	Unit	Source
gf	-489.17	kJ/mol	Joback Method
hf	-882.07	kJ/mol	Joback Method
hfus	45.90	kJ/mol	Joback Method
hvap	78.92	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.678		Crippen Method
mvol	255.520	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
tb	814.28	K	Joback Method
tc	1014.35	K	Joback Method
tf	507.64	K	Joback Method
vc	0.995	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.88	J/molxK	814.28	Joback Method
cpg	751.62	J/molxK	847.62	Joback Method
cpg	764.38	J/molxK	880.97	Joback Method
cpg	776.17	J/molxK	914.31	Joback Method
cpg	787.02	J/molxK	947.66	Joback Method
cpg	796.92	J/molxK	981.00	Joback Method
cpg	805.90	J/molxK	1014.35	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=U391514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391514&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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