

# Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-fluoro-2-methoxyphenyl ester

Inchi:	InChI=1S/C15H15F5O5/c1-23-11-7-9(16)5-6-10(11)25-13(22)4-2-3-12(21)24-8-15(19,20
InchiKey:	BPDMKLZXXNNQLV-UHFFFAOYSA-N
Formula:	C15H15F5O5
SMILES:	COc1cc(F)ccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	370.27

## Physical Properties

Property code	Value	Unit	Source
gf	-1377.92	kJ/mol	Joback Method
hf	-1755.74	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	67.54	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.354		Crippen Method
mvol	228.050	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook
tb	746.92	K	Joback Method
tc	930.93	K	Joback Method
tf	467.19	K	Joback Method
vc	0.906	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.53	J/molxK	746.92	Joback Method
cpg	673.87	J/molxK	777.59	Joback Method
cpg	685.39	J/molxK	808.26	Joback Method
cpg	696.11	J/molxK	838.93	Joback Method
cpg	706.02	J/molxK	869.60	Joback Method
cpg	715.14	J/molxK	900.26	Joback Method
cpg	723.49	J/molxK	930.93	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=U393435&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393435&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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