

# Glutaric acid, but-3-en-2-yl 2,2,3,3-tetrafluoropropyl ester

<b>Inchi:</b>	InChI=1S/C12H16F4O4/c1-3-8(2)20-10(18)6-4-5-9(17)19-7-12(15,16)11(13)14/h3,8,11H
<b>InchiKey:</b>	VKMWOWBFIOROJH-UHFFFAOYSA-N
<b>Formula:</b>	C12H16F4O4
<b>SMILES:</b>	<chem>C=CC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)F</chem>
<b>Mol. weight [g/mol]:</b>	300.25

## Physical Properties

Property code	Value	Unit	Source
gf	-1111.12	kJ/mol	Joback Method
hf	-1458.93	kJ/mol	Joback Method
hfus	28.99	kJ/mol	Joback Method
hvap	54.61	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.718		Crippen Method
mvol	197.600	ml/mol	McGowan Method
pc	1763.93	kPa	Joback Method
rinpol	1373.00		NIST Webbook
rinpol	1373.00		NIST Webbook
tb	616.19	K	Joback Method
tc	783.81	K	Joback Method
tf	342.34	K	Joback Method
vc	0.785	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.42	J/mol×K	616.19	Joback Method
cpg	543.29	J/mol×K	644.13	Joback Method
cpg	555.52	J/mol×K	672.06	Joback Method
cpg	567.12	J/mol×K	700.00	Joback Method
cpg	578.09	J/mol×K	727.94	Joback Method
cpg	588.47	J/mol×K	755.87	Joback Method
cpg	598.25	J/mol×K	783.81	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<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=U405231&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405231&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>

# 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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