

# Glutaric acid, 2,2,3,3-tetrafluoropropyl non-5-yn-3-yl ester

<b>Inchi:</b>	InChI=1S/C17H24F4O4/c1-3-5-6-7-9-13(4-2)25-15(23)11-8-10-14(22)24-12-17(20,21)16
<b>InchiKey:</b>	MQMUQGMKRRZIBE-UHFFFAOYSA-N
<b>Formula:</b>	C17H24F4O4
<b>SMILES:</b>	CCCC#CCC(CC)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	368.36

## Physical Properties

Property code	Value	Unit	Source
gf	-954.06	kJ/mol	Joback Method
hf	-1415.26	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.116		Crippen Method
mvol	263.750	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	1844.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tb	742.91	K	Joback Method
tc	922.12	K	Joback Method
tf	506.55	K	Joback Method
vc	1.046	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.21	J/mol×K	742.91	Joback Method
cpg	793.24	J/mol×K	772.78	Joback Method
cpg	807.40	J/mol×K	802.65	Joback Method
cpg	820.74	J/mol×K	832.51	Joback Method
cpg	833.26	J/mol×K	862.38	Joback Method
cpg	845.00	J/mol×K	892.25	Joback Method
cpg	855.97	J/mol×K	922.12	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393949&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>hvp:</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>rinp:</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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