

# Glutaric acid, 1,1,1-trifluoroprop-2-yl oct-3-en-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H25F3O4/c1-4-5-6-7-9-12(2)22-14(20)10-8-11-15(21)23-13(3)16(17,18)19
<b>InchiKey:</b>	PBYLROOOKDHVAP-VQHVLOKHSA-N
<b>Formula:</b>	C16H25F3O4
<b>SMILES:</b>	CCCCC=CC(C)OC(=O)CCCC(=O)OC(C)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	338.36

## Physical Properties

Property code	Value	Unit	Source
gf	-890.25	kJ/mol	Joback Method
hf	-1353.59	kJ/mol	Joback Method
hfus	37.75	kJ/mol	Joback Method
hvap	64.96	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.329		Crippen Method
mcvol	252.190	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	715.92	K	Joback Method
tc	891.85	K	Joback Method
tf	383.51	K	Joback Method
vc	0.991	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.88	J/mol×K	715.92	Joback Method
cpg	752.14	J/mol×K	745.24	Joback Method
cpg	766.58	J/mol×K	774.56	Joback Method
cpg	780.22	J/mol×K	803.88	Joback Method
cpg	793.09	J/mol×K	833.20	Joback Method
cpg	805.21	J/mol×K	862.52	Joback Method
cpg	816.62	J/mol×K	891.85	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U393981&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393981&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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