

# Glutaric acid, hex-2-en-1-yl 1,1,1-trifluoroprop-2-yl ester

Inchi:	InChI=1S/C14H21F3O4/c1-3-4-5-6-10-20-12(18)8-7-9-13(19)21-11(2)14(15,16)17/h5-6,1
InchiKey:	YQNKPNMKJMFEOE-AATRIKPKSA-N
Formula:	C14H21F3O4
SMILES:	CCCC=CCOC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]:	310.31

## Physical Properties

Property code	Value	Unit	Source
gf	-904.65	kJ/mol	Joback Method
hf	-1307.03	kJ/mol	Joback Method
hfus	36.09	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.550		Crippen Method
mvol	224.010	ml/mol	McGowan Method
pc	1567.23	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1540.00		NIST Webbook
tb	670.60	K	Joback Method
tc	843.97	K	Joback Method
tf	375.97	K	Joback Method
vc	0.884	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.05	J/mol×K	670.60	Joback Method
cpg	641.24	J/mol×K	699.50	Joback Method
cpg	654.68	J/mol×K	728.39	Joback Method
cpg	667.42	J/mol×K	757.29	Joback Method
cpg	679.45	J/mol×K	786.18	Joback Method
cpg	690.82	J/mol×K	815.08	Joback Method
cpg	701.54	J/mol×K	843.97	Joback Method

# Sources

<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=U405323&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405323&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.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>

# 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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