

# Glutaric acid, hexa-1,5-dien-3-yl 1,1,1-trifluoroprop-2-yl ester

Inchi:	InChI=1S/C14H19F3O4/c1-4-7-11(5-2)21-13(19)9-6-8-12(18)20-10(3)14(15,16)17/h4-5,1
InchiKey:	LIEUNBMBZIHMHY-UHFFFAOYSA-N
Formula:	C14H19F3O4
SMILES:	<chem>C=CCC(C=C)OC(=O)CCCC(=O)OC(C)C(F)(F)F</chem>
Mol. weight [g/mol]:	308.29

## Physical Properties

Property code	Value	Unit	Source
gf	-811.63	kJ/mol	Joback Method
hf	-1178.67	kJ/mol	Joback Method
hfus	29.81	kJ/mol	Joback Method
hvap	59.21	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.325		Crippen Method
mvol	219.710	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
tb	659.36	K	Joback Method
tc	834.04	K	Joback Method
tf	362.53	K	Joback Method
vc	0.861	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.53	J/molxK	659.36	Joback Method
cpg	617.39	J/molxK	688.47	Joback Method
cpg	630.50	J/molxK	717.59	Joback Method
cpg	642.89	J/molxK	746.70	Joback Method
cpg	654.57	J/molxK	775.81	Joback Method
cpg	665.57	J/molxK	804.93	Joback Method
cpg	675.92	J/molxK	834.04	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405271&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405271&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.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>

# 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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