

# Glutaric acid, octadecyl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi:	InChI=1S/C31H49F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-26-37-28(35)24-21
InchiKey:	RLQDPNARUAYDDE-UHFFFAOYSA-N
Formula:	C31H49F3O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	542.71

## Physical Properties

Property code	Value	Unit	Source
gf	-729.32	kJ/mol	Joback Method
hf	-1538.60	kJ/mol	Joback Method
hfus	73.96	kJ/mol	Joback Method
hvap	101.05	kJ/mol	Joback Method
log10ws	-10.75		Crippen Method
logp	9.808		Crippen Method
mvol	444.080	ml/mol	McGowan Method
pc	664.60	kPa	Joback Method
rinpol	3402.00		NIST Webbook
rinpol	3402.00		NIST Webbook
tb	1082.08	K	Joback Method
tc	1353.16	K	Joback Method
tf	599.06	K	Joback Method
vc	1.748	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1581.01	J/molxK	1082.08	Joback Method
cpg	1601.28	J/molxK	1127.26	Joback Method
cpg	1619.53	J/molxK	1172.44	Joback Method
cpg	1635.94	J/molxK	1217.62	Joback Method
cpg	1650.71	J/molxK	1262.80	Joback Method
cpg	1664.02	J/molxK	1307.98	Joback Method
cpg	1676.06	J/molxK	1353.16	Joback Method

# Sources

<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=U377380&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377380&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>

# 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>hvap:</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>rinpola:</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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