

# Glutaric acid, 2,2,2-trifluoroethyl hexadecyl ester

Inchi:	InChI=1S/C23H41F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-29-21(27)17-16-18-22
InchiKey:	JJDAXNHLYMQDEN-UHFFFAOYSA-N
Formula:	C23H41F3O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]:	438.56

## Physical Properties

Property code	Value	Unit	Source
gf	-906.65	kJ/mol	Joback Method
hf	-1604.73	kJ/mol	Joback Method
hfus	62.73	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.287		Crippen Method
mcvol	355.120	ml/mol	McGowan Method
pc	840.16	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	872.80	K	Joback Method
tc	1070.68	K	Joback Method
tf	497.48	K	Joback Method
vc	1.415	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.26	J/mol×K	872.80	Joback Method
cpg	1195.49	J/mol×K	905.78	Joback Method
cpg	1213.46	J/mol×K	938.76	Joback Method
cpg	1230.22	J/mol×K	971.74	Joback Method
cpg	1245.80	J/mol×K	1004.72	Joback Method
cpg	1260.26	J/mol×K	1037.70	Joback Method
cpg	1273.65	J/mol×K	1070.68	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380523&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380523&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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