

# Glutaric acid, 2,2,3,3,4,4,4-heptafluorobutyl tridecyl ester

Inchi:	InChI=1S/C22H35F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-32-18(30)14-13-15-19(31)33-17
InchiKey:	WGPUNPSNOQWQMM-UHFFFAOYSA-N
Formula:	C22H35F7O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	496.50

## Physical Properties

Property code	Value	Unit	Source
gf	-1688.63	kJ/mol	Joback Method
hf	-2386.03	kJ/mol	Joback Method
hfus	57.63	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.387		Crippen Method
mcvol	348.110	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpola	2461.00		NIST Webbook
rinpola	2461.00		NIST Webbook
tb	840.54	K	Joback Method
tc	1031.22	K	Joback Method
tf	493.41	K	Joback Method
vc	1.409	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1144.76	J/molxK	840.54	Joback Method
cpg	1162.51	J/molxK	872.32	Joback Method
cpg	1179.14	J/molxK	904.10	Joback Method
cpg	1194.72	J/molxK	935.88	Joback Method
cpg	1209.33	J/molxK	967.66	Joback Method
cpg	1223.03	J/molxK	999.44	Joback Method
cpg	1235.91	J/molxK	1031.22	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=U377558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377558&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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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