

# Glutaric acid, 2,3,4,5-tetrafluorobenzyl tridecyl ester

Inchi:	InChI=1S/C25H36F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-32-21(30)14-13-15-22(31)33-18
InchiKey:	KYZRNFQVDDYFLM-UHFFFAOYSA-N
Formula:	C25H36F4O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	476.54

## Physical Properties

Property code	Value	Unit	Source
gf	-1013.57	kJ/mol	Joback Method
hf	-1642.72	kJ/mol	Joback Method
hfus	70.89	kJ/mol	Joback Method
hvap	91.21	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.311		Crippen Method
mvol	361.310	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	2951.00		NIST Webbook
rinpol	2951.00		NIST Webbook
tb	967.66	K	Joback Method
tc	1191.37	K	Joback Method
tf	594.69	K	Joback Method
vc	1.448	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.00	J/molxK	967.66	Joback Method
cpg	1223.88	J/molxK	1004.95	Joback Method
cpg	1239.14	J/molxK	1042.23	Joback Method
cpg	1252.81	J/molxK	1079.52	Joback Method
cpg	1264.93	J/molxK	1116.80	Joback Method
cpg	1275.52	J/molxK	1154.09	Joback Method
cpg	1284.63	J/molxK	1191.37	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=U377451&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377451&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>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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