

# Glutaric acid, tridecyl 2,3,6-trifluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C25H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-31-23(29)14-13-15-24(30)32-19
<b>InchiKey:</b>	IELIOYPKYJQRHG-UHFFFAOYSA-N
<b>Formula:</b>	C25H37F3O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	458.55

## Physical Properties

Property code	Value	Unit	Source
gf	-809.13	kJ/mol	Joback Method
hf	-1435.14	kJ/mol	Joback Method
hfus	68.19	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.172		Crippen Method
mvol	359.540	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	963.41	K	Joback Method
tc	1183.18	K	Joback Method
tf	581.58	K	Joback Method
vc	1.429	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.79	J/molxK	963.41	Joback Method
cpg	1217.72	J/molxK	1000.04	Joback Method
cpg	1233.10	J/molxK	1036.67	Joback Method
cpg	1246.97	J/molxK	1073.29	Joback Method
cpg	1259.36	J/molxK	1109.92	Joback Method
cpg	1270.32	J/molxK	1146.55	Joback Method
cpg	1279.87	J/molxK	1183.18	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=U376905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376905&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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