

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

<b>Inchi:</b>	InChI=1S/C24H35F3O4/c1-2-3-4-5-6-7-8-9-10-11-17-30-22(28)13-12-14-23(29)31-18-19
<b>InchiKey:</b>	QGTWGRVGLJESF-UHFFFAOYSA-N
<b>Formula:</b>	C24H35F3O4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	444.53

## Physical Properties

Property code	Value	Unit	Source
gf	-817.55	kJ/mol	Joback Method
hf	-1414.50	kJ/mol	Joback Method
hfus	65.60	kJ/mol	Joback Method
hvap	89.14	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	6.782		Crippen Method
mvol	345.450	ml/mol	McGowan Method
pc	930.07	kPa	Joback Method
rinpol	2853.00		NIST Webbook
rinpol	2853.00		NIST Webbook
tb	940.53	K	Joback Method
tc	1152.88	K	Joback Method
tf	570.31	K	Joback Method
vc	1.373	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.20	J/molxK	940.53	Joback Method
cpg	1155.70	J/molxK	975.92	Joback Method
cpg	1170.78	J/molxK	1011.31	Joback Method
cpg	1184.48	J/molxK	1046.71	Joback Method
cpg	1196.81	J/molxK	1082.10	Joback Method
cpg	1207.82	J/molxK	1117.49	Joback Method
cpg	1217.53	J/molxK	1152.88	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=U376904&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376904&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>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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