

# Glutaric acid, 2,4,5-trifluorobenzyl 2-methylhex-3-yl ester

<b>Inchi:</b>	InChI=1S/C19H25F3O4/c1-4-6-17(12(2)3)26-19(24)8-5-7-18(23)25-11-13-9-15(21)16(22)
<b>InchiKey:</b>	JVTUIGPMRPBRBT-UHFFFAOYSA-N
<b>Formula:</b>	C19H25F3O4
<b>SMILES:</b>	CCCC(OC(=O)CCCC(=O)OCc1cc(F)c(F)cc1F)C(C)C
<b>Mol. weight [g/mol]:</b>	374.39

## Physical Properties

Property code	Value	Unit	Source
gf	-864.53	kJ/mol	Joback Method
hf	-1321.86	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.685		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	2426.00		NIST Webbook
rinpol	2426.00		NIST Webbook
tb	825.25	K	Joback Method
tc	1017.82	K	Joback Method
tf	483.96	K	Joback Method
vc	1.081	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.06	J/mol×K	825.25	Joback Method
cpg	855.83	J/mol×K	857.35	Joback Method
cpg	869.58	J/mol×K	889.44	Joback Method
cpg	882.31	J/mol×K	921.54	Joback Method
cpg	894.04	J/mol×K	953.63	Joback Method
cpg	904.78	J/mol×K	985.73	Joback Method
cpg	914.53	J/mol×K	1017.82	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=U380463&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380463&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>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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