

# Glutaric acid, 2-methylhex-3-yl 2-(trifluoromethyl)benzyl ester

<b>Inchi:</b>	InChI=1S/C20H27F3O4/c1-4-8-17(14(2)3)27-19(25)12-7-11-18(24)26-13-15-9-5-6-10-16
<b>InchiKey:</b>	HNKCEQSGYBRDPU-UHFFFAOYSA-N
<b>Formula:</b>	C20H27F3O4
<b>SMILES:</b>	CCCC(OC(=O)CCCC(=O)OCc1cccc1C(F)(F)F)C(C)C
<b>Mol. weight [g/mol]:</b>	388.42

## Physical Properties

Property code	Value	Unit	Source
gf	-834.01	kJ/mol	Joback Method
hf	-1328.31	kJ/mol	Joback Method
hfus	41.56	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.287		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	834.94	K	Joback Method
tc	1030.90	K	Joback Method
tf	472.61	K	Joback Method
vc	1.127	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.96	J/molxK	834.94	Joback Method
cpg	917.22	J/molxK	867.60	Joback Method
cpg	931.40	J/molxK	900.26	Joback Method
cpg	944.52	J/molxK	932.92	Joback Method
cpg	956.65	J/molxK	965.58	Joback Method
cpg	967.80	J/molxK	998.24	Joback Method
cpg	978.03	J/molxK	1030.90	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<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=U377492&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377492&amp;Units=SI</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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