

# Glutaric acid, butyl 4-(trifluoromethyl)benzyl ester

Inchi:	InChI=1S/C17H21F3O4/c1-2-3-11-23-15(21)5-4-6-16(22)24-12-13-7-9-14(10-8-13)17(18)
InchiKey:	UMFTVQYRFPQJQD-UHFFFAOYSA-N
Formula:	C17H21F3O4
SMILES:	CCCCOC(=O)CCCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	346.34

## Physical Properties

Property code	Value	Unit	Source
gf	-854.39	kJ/mol	Joback Method
hf	-1255.83	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.262		Crippen Method
mvol	246.820	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	767.18	K	Joback Method
tc	957.59	K	Joback Method
tf	468.80	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.19	J/mol×K	767.18	Joback Method
cpg	743.32	J/mol×K	798.92	Joback Method
cpg	756.53	J/mol×K	830.65	Joback Method
cpg	768.84	J/mol×K	862.39	Joback Method
cpg	780.28	J/mol×K	894.12	Joback Method
cpg	790.87	J/mol×K	925.86	Joback Method
cpg	800.66	J/mol×K	957.59	Joback Method

# Sources

<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>
<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=U377579&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377579&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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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

Latest version available from:

<https://www.chemeo.com/cid/55-340-3/Glutaric-acid-butyl-4-trifluoromethyl-benzyl-ester.pdf>

Generated by Cheméo on 2025-12-05 19:15:26.441461325 +0000 UTC m=+4710323.971501980.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.