

# Glutaric acid, butyl 3,4-difluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C16H20F2O4/c1-2-3-9-21-15(19)5-4-6-16(20)22-11-12-7-8-13(17)14(18)10-12
<b>InchiKey:</b>	CCWUSAQOLGNRSN-UHFFFAOYSA-N
<b>Formula:</b>	C16H20F2O4
<b>SMILES:</b>	CCCCOC(=O)CCCC(=O)OCc1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	314.32

## Physical Properties

Property code	Value	Unit	Source
gf	-680.47	kJ/mol	Joback Method
hf	-1041.80	kJ/mol	Joback Method
hfus	42.19	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.522		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinqol	2256.00		NIST Webbook
tb	753.24	K	Joback Method
tc	943.80	K	Joback Method
tf	467.04	K	Joback Method
vc	0.907	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.08	J/mol×K	753.24	Joback Method
cpg	677.05	J/mol×K	785.00	Joback Method
cpg	690.16	J/mol×K	816.76	Joback Method
cpg	702.41	J/mol×K	848.52	Joback Method
cpg	713.82	J/mol×K	880.28	Joback Method
cpg	724.40	J/mol×K	912.04	Joback Method
cpg	734.14	J/mol×K	943.80	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377635&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377635&amp;Units=SI</a>
<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>

# 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>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

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