

# Glutaric acid, tridec-2-yn-1-yl 2-bromo-4-fluorophenyl ester

<b>Inchi:</b>	InChI=1S/C24H32BrFO4/c1-2-3-4-5-6-7-8-9-10-11-12-18-29-23(27)14-13-15-24(28)30-2
<b>InchiKey:</b>	LEQLPUHRFBFQTG-UHFFFAOYSA-N
<b>Formula:</b>	C24H32BrFO4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(F)cc1Br
<b>Mol. weight [g/mol]:</b>	483.41

## Physical Properties

Property code	Value	Unit	Source
gf	-201.18	kJ/mol	Joback Method
hf	-712.18	kJ/mol	Joback Method
hfus	68.24	kJ/mol	Joback Method
hvap	98.70	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	6.741		Crippen Method
mcvol	350.810	ml/mol	McGowan Method
pc	1153.00	kPa	Joback Method
rinsol	3122.00		NIST Webbook
tb	1012.17	K	Joback Method
tc	1239.63	K	Joback Method
tf	722.51	K	Joback Method
vc	1.361	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.72	J/molxK	1012.17	Joback Method
cpg	1121.61	J/molxK	1050.08	Joback Method
cpg	1134.15	J/molxK	1087.99	Joback Method
cpg	1145.39	J/molxK	1125.90	Joback Method
cpg	1155.36	J/molxK	1163.81	Joback Method
cpg	1164.12	J/molxK	1201.72	Joback Method
cpg	1171.71	J/molxK	1239.63	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391841&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391841&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>mccvol:</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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