

# Glutaric acid, 2-bromo-5-fluorobenzyl nonyl ester

<b>Inchi:</b>	InChI=1S/C21H30BrFO4/c1-2-3-4-5-6-7-8-14-26-20(24)10-9-11-21(25)27-16-17-15-18(2
<b>InchiKey:</b>	BJYMOZAOBLBNLW-UHFFFAOYSA-N
<b>Formula:</b>	C21H30BrFO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
<b>Mol. weight [g/mol]:</b>	445.36

## Physical Properties

Property code	Value	Unit	Source
gf	-429.24	kJ/mol	Joback Method
hf	-922.56	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.096		Crippen Method
mcvol	317.140	ml/mol	McGowan Method
pc	1260.16	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	934.53	K	Joback Method
tc	1146.38	K	Joback Method
tf	582.60	K	Joback Method
vc	1.232	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.74	J/molxK	934.53	Joback Method
cpg	998.04	J/molxK	969.84	Joback Method
cpg	1011.15	J/molxK	1005.15	Joback Method
cpg	1023.11	J/molxK	1040.46	Joback Method
cpg	1033.94	J/molxK	1075.77	Joback Method
cpg	1043.69	J/molxK	1111.07	Joback Method
cpg	1052.38	J/molxK	1146.38	Joback Method

# Sources

<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=U377068&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377068&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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