

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

<b>Inchi:</b>	InChI=1S/C28H44BrFO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-33-27(31)17-16-18-2
<b>InchiKey:</b>	KGKZHIAYOWWGOW-UHFFFAOYSA-N
<b>Formula:</b>	C28H44BrFO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
<b>Mol. weight [g/mol]:</b>	543.55

## Physical Properties

Property code	Value	Unit	Source
gf	-370.30	kJ/mol	Joback Method
hf	-1067.04	kJ/mol	Joback Method
hfus	75.48	kJ/mol	Joback Method
hvap	105.45	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.826		Crippen Method
mvol	415.770	ml/mol	McGowan Method
pc	821.48	kPa	Joback Method
rinpol	3554.00		NIST Webbook
rinpol	3554.00		NIST Webbook
tb	1094.69	K	Joback Method
tc	1354.30	K	Joback Method
tf	661.49	K	Joback Method
vc	1.623	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1413.85	J/molxK	1094.69	Joback Method
cpg	1430.41	J/molxK	1137.96	Joback Method
cpg	1445.07	J/molxK	1181.23	Joback Method
cpg	1457.93	J/molxK	1224.50	Joback Method
cpg	1469.08	J/molxK	1267.76	Joback Method
cpg	1478.64	J/molxK	1311.03	Joback Method
cpg	1486.69	J/molxK	1354.30	Joback Method

# Sources

<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=U376864&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376864&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>

# 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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