

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

Inchi:	InChI=1S/C25H38BrFO4/c1-2-3-4-5-6-7-8-9-10-11-12-18-30-24(28)14-13-15-25(29)31-2
InchiKey:	GCAXNPDPZPXQNK-UHFFFAOYSA-N
Formula:	C25H38BrFO4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	501.47

## Physical Properties

Property code	Value	Unit	Source
gf	-395.56	kJ/mol	Joback Method
hf	-1005.12	kJ/mol	Joback Method
hfus	67.71	kJ/mol	Joback Method
hvap	98.77	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.656		Crippen Method
mvol	373.500	ml/mol	McGowan Method
pc	975.95	kPa	Joback Method
rinpol	3237.00		NIST Webbook
rinpol	3237.00		NIST Webbook
tb	1026.05	K	Joback Method
tc	1258.11	K	Joback Method
tf	627.68	K	Joback Method
vc	1.456	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.96	J/molxK	1026.05	Joback Method
cpg	1242.40	J/molxK	1064.73	Joback Method
cpg	1256.33	J/molxK	1103.40	Joback Method
cpg	1268.81	J/molxK	1142.08	Joback Method
cpg	1279.90	J/molxK	1180.76	Joback Method
cpg	1289.65	J/molxK	1219.44	Joback Method
cpg	1298.13	J/molxK	1258.11	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=U376861&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376861&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.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>

# 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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