

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

Inchi:	InChI=1S/C20H28BrFO4/c1-2-3-4-5-6-7-13-25-19(23)9-8-10-20(24)26-15-16-14-17(22)1
InchiKey:	DJOXHFCDVWBFQQ-UHFFFAOYSA-N
Formula:	C20H28BrFO4
SMILES:	CCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1Br
Mol. weight [g/mol]:	431.34

## Physical Properties

Property code	Value	Unit	Source
gf	-437.66	kJ/mol	Joback Method
hf	-901.92	kJ/mol	Joback Method
hfus	54.76	kJ/mol	Joback Method
hvap	87.64	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.705		Crippen Method
mvol	303.050	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2719.00		NIST Webbook
rinpol	2719.00		NIST Webbook
tb	911.65	K	Joback Method
tc	1120.89	K	Joback Method
tf	571.33	K	Joback Method
vc	1.175	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.33	J/molxK	911.65	Joback Method
cpg	938.37	J/molxK	946.52	Joback Method
cpg	951.28	J/molxK	981.40	Joback Method
cpg	963.10	J/molxK	1016.27	Joback Method
cpg	973.84	J/molxK	1051.14	Joback Method
cpg	983.54	J/molxK	1086.02	Joback Method
cpg	992.22	J/molxK	1120.89	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=U377067&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377067&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>h vap:</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>r in pol:</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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