

# Glutaric acid, 2,6-difluoro-4-bromobenzyl octyl ester

<b>Inchi:</b>	InChI=1S/C20H27BrF2O4/c1-2-3-4-5-6-7-11-26-19(24)9-8-10-20(25)27-14-16-17(22)12-
<b>InchiKey:</b>	AHGUMLLRMIWPRD-UHFFFAOYSA-N
<b>Formula:</b>	C20H27BrF2O4
<b>SMILES:</b>	CCCCCCCCOC(=O)CCCC(=O)OCc1c(F)cc(Br)cc1F
<b>Mol. weight [g/mol]:</b>	449.33

## Physical Properties

Property code	Value	Unit	Source
gf	-642.10	kJ/mol	Joback Method
hf	-1109.50	kJ/mol	Joback Method
hfus	57.45	kJ/mol	Joback Method
hvap	87.49	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.845		Crippen Method
mcvol	304.820	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinqol	2689.00		NIST Webbook
tb	915.90	K	Joback Method
tc	1123.72	K	Joback Method
tf	584.44	K	Joback Method
vc	1.194	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.46	J/molxK	915.90	Joback Method
cpg	944.14	J/molxK	950.54	Joback Method
cpg	956.71	J/molxK	985.17	Joback Method
cpg	968.18	J/molxK	1019.81	Joback Method
cpg	978.57	J/molxK	1054.45	Joback Method
cpg	987.91	J/molxK	1089.09	Joback Method
cpg	996.23	J/molxK	1123.72	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=U376824&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376824&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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