

# Glutaric acid, 2-bromobenzyl nonyl ester

<b>Inchi:</b>	InChI=1S/C21H31BrO4/c1-2-3-4-5-6-7-10-16-25-20(23)14-11-15-21(24)26-17-18-12-8-9
<b>InchiKey:</b>	ODJNKOFPLAOVCB-UHFFFAOYSA-N
<b>Formula:</b>	C21H31BrO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCCC(=O)OCc1ccccc1Br
<b>Mol. weight [g/mol]:</b>	427.37

## Physical Properties

Property code	Value	Unit	Source
gf	-224.80	kJ/mol	Joback Method
hf	-714.98	kJ/mol	Joback Method
hfus	54.66	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	5.956		Crippen Method
mvol	315.370	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2872.00		NIST Webbook
tb	930.28	K	Joback Method
tc	1143.52	K	Joback Method
tf	569.49	K	Joback Method
vc	1.214	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.64	J/molxK	930.28	Joback Method
cpg	992.30	J/molxK	965.82	Joback Method
cpg	1005.78	J/molxK	1001.36	Joback Method
cpg	1018.09	J/molxK	1036.90	Joback Method
cpg	1029.29	J/molxK	1072.44	Joback Method
cpg	1039.42	J/molxK	1107.98	Joback Method
cpg	1048.51	J/molxK	1143.52	Joback Method
dvisc	0.0003471	Paxs	569.49	Joback Method
dvisc	0.0001999	Paxs	629.62	Joback Method

dvisc	0.0001267	Paxs	689.75	Joback Method
dvisc	0.0000864	Paxs	749.88	Joback Method
dvisc	0.0000624	Paxs	810.02	Joback Method
dvisc	0.0000471	Paxs	870.15	Joback Method
dvisc	0.0000369	Paxs	930.28	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=U376767&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376767&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>dvisc:</b>	Dynamic viscosity
<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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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