

# Glutaric acid, 2-bromobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C19H27BrO4/c1-4-8-17(14(2)3)24-19(22)12-7-11-18(21)23-13-15-9-5-6-10-16
InchiKey:	GXQZLNLMRITSC-UHFFFAOYSA-N
Formula:	C19H27BrO4
SMILES:	CCCC(OC(=O)CCCC(=O)OCc1ccccc1Br)C(C)C
Mol. weight [g/mol]:	399.32

## Physical Properties

Property code	Value	Unit	Source
gf	-246.52	kJ/mol	Joback Method
hf	-684.26	kJ/mol	Joback Method
hfus	42.43	kJ/mol	Joback Method
hvap	84.80	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.030		Crippen Method
mvol	287.190	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	883.64	K	Joback Method
tc	1098.00	K	Joback Method
tf	516.95	K	Joback Method
vc	1.089	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.39	J/molxK	883.64	Joback Method
cpg	874.83	J/molxK	919.37	Joback Method
cpg	888.10	J/molxK	955.09	Joback Method
cpg	900.24	J/molxK	990.82	Joback Method
cpg	911.27	J/molxK	1026.55	Joback Method
cpg	921.22	J/molxK	1062.27	Joback Method
cpg	930.14	J/molxK	1098.00	Joback Method
dvisc	0.0005344	Paxs	516.95	Joback Method

dvisc	0.0002789	Paxs	578.07	Joback Method
dvisc	0.0001649	Paxs	639.18	Joback Method
dvisc	0.0001068	Paxs	700.30	Joback Method
dvisc	0.0000742	Paxs	761.41	Joback Method
dvisc	0.0000544	Paxs	822.52	Joback Method
dvisc	0.0000417	Paxs	883.64	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=U376763&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376763&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>mcvol:</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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