

# Glutaric acid, 2-(4-bromophenyl)ethyl hexyl ester

Inchi:	InChI=1S/C19H27BrO4/c1-2-3-4-5-14-23-18(21)7-6-8-19(22)24-15-13-16-9-11-17(20)12
InchiKey:	BZETXCVQWSVHTD-UHFFFAOYSA-N
Formula:	C19H27BrO4
SMILES:	CCCCCOC(=O)CCCC(=O)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	399.32

## Physical Properties

Property code	Value	Unit	Source
gf	-241.64	kJ/mol	Joback Method
hf	-673.70	kJ/mol	Joback Method
hfus	49.48	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.829		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpola	2756.00		NIST Webbook
rinpola	2756.00		NIST Webbook
tb	884.52	K	Joback Method
tc	1095.03	K	Joback Method
tf	546.95	K	Joback Method
vc	1.101	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.35	J/molxK	884.52	Joback Method
cpg	919.80	J/molxK	1059.94	Joback Method
cpg	909.80	J/molxK	1024.86	Joback Method
cpg	898.78	J/molxK	989.77	Joback Method
cpg	886.72	J/molxK	954.69	Joback Method
cpg	873.59	J/molxK	919.60	Joback Method
cpg	928.82	J/molxK	1095.03	Joback Method
dvisc	0.0000498	Paxs	884.52	Joback Method

dvisc	0.0000632	Paxs	828.26	Joback Method
dvisc	0.0000831	Paxs	772.00	Joback Method
dvisc	0.0001139	Paxs	715.73	Joback Method
dvisc	0.0001649	Paxs	659.47	Joback Method
dvisc	0.0002558	Paxs	603.21	Joback Method
dvisc	0.0004342	Paxs	546.95	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377357&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377357&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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