

# Glutaric acid, 2-(3-bromophenyl)ethyl ethyl ester

Inchi:	InChI=1S/C15H19BrO4/c1-2-19-14(17)7-4-8-15(18)20-10-9-12-5-3-6-13(16)11-12/h3,5-6
InchiKey:	CQEJULHLZQKSTC-UHFFFAOYSA-N
Formula:	C15H19BrO4
SMILES:	CCOC(=O)CCCC(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]:	343.21

## Physical Properties

Property code	Value	Unit	Source
gf	-275.32	kJ/mol	Joback Method
hf	-591.14	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	76.67	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.268		Crippen Method
mcvol	230.830	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinqol	2292.00		NIST Webbook
tb	793.00	K	Joback Method
tc	1006.77	K	Joback Method
tf	501.87	K	Joback Method
vc	0.877	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.16	J/molxK	793.00	Joback Method
cpg	645.38	J/molxK	828.63	Joback Method
cpg	657.63	J/molxK	864.26	Joback Method
cpg	668.93	J/molxK	899.88	Joback Method
cpg	679.29	J/molxK	935.51	Joback Method
cpg	688.74	J/molxK	971.14	Joback Method
cpg	697.29	J/molxK	1006.77	Joback Method
dvisc	0.0006502	Paxs	501.87	Joback Method
dvisc	0.0004028	Paxs	550.39	Joback Method

dvisc	0.0002696	Paxs	598.91	Joback Method
dvisc	0.0001917	Paxs	647.43	Joback Method
dvisc	0.0001429	Paxs	695.96	Joback Method
dvisc	0.0001107	Paxs	744.48	Joback Method
dvisc	0.0000885	Paxs	793.00	Joback Method

## Sources

<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>
<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=U377203&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377203&amp;Units=SI</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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