

# Glutaric acid, 7-bromoheptyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H33BrO4/c1-4-16(15(2)3)23-18(21)12-10-11-17(20)22-14-9-7-5-6-8-13-19
InchiKey:	BLLVRNOIAKPUJC-UHFFFAOYSA-N
Formula:	C18H33BrO4
SMILES:	CCC(OC(=O)CCCC(=O)OCCCCCBr)C(C)C
Mol. weight [g/mol]:	393.36

## Physical Properties

Property code	Value	Unit	Source
gf	-357.72	kJ/mol	Joback Method
hf	-888.68	kJ/mol	Joback Method
hfus	46.19	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.023		Crippen Method
mcvol	296.860	ml/mol	McGowan Method
pc	1304.23	kPa	Joback Method
rinpola	2504.00		NIST Webbook
rinpola	2504.00		NIST Webbook
tb	829.10	K	Joback Method
tc	1022.40	K	Joback Method
tf	466.74	K	Joback Method
vc	1.141	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.14	J/molxK	829.10	Joback Method
cpg	914.43	J/molxK	861.32	Joback Method
cpg	929.70	J/molxK	893.53	Joback Method
cpg	943.97	J/molxK	925.75	Joback Method
cpg	957.25	J/molxK	957.96	Joback Method
cpg	969.58	J/molxK	990.18	Joback Method
cpg	980.97	J/molxK	1022.40	Joback Method
dvisc	0.0008566	Paxs	466.74	Joback Method

dvisc	0.0004000	Paxs	527.13	Joback Method
dvisc	0.0002184	Paxs	587.53	Joback Method
dvisc	0.0001335	Paxs	647.92	Joback Method
dvisc	0.0000888	Paxs	708.31	Joback Method
dvisc	0.0000629	Paxs	768.71	Joback Method
dvisc	0.0000469	Paxs	829.10	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=U380504&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380504&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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