

# Glutaric acid, 7-chloroheptyl 7-bromoheptyl ester

Inchi:	InChI=1S/C19H34BrClO4/c20-14-7-3-1-5-9-16-24-18(22)12-11-13-19(23)25-17-10-6-2-4
InchiKey:	QEMNZYNCLQURJG-UHFFFAOYSA-N
Formula:	C19H34BrClO4
SMILES:	O=C(CCCC(=O)OCCCCCBr)OCCCCCCCCI
Mol. weight [g/mol]:	441.83

## Physical Properties

Property code	Value	Unit	Source
gf	-356.35	kJ/mol	Joback Method
hf	-914.50	kJ/mol	Joback Method
hfus	60.02	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.778		Crippen Method
mvol	323.190	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2960.00		NIST Webbook
rinpol	2960.00		NIST Webbook
tb	890.29	K	Joback Method
tc	1091.00	K	Joback Method
tf	537.93	K	Joback Method
vc	1.258	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.87	J/molxK	890.29	Joback Method
cpg	1000.43	J/molxK	923.74	Joback Method
cpg	1014.92	J/molxK	957.19	Joback Method
cpg	1028.36	J/molxK	990.64	Joback Method
cpg	1040.78	J/molxK	1024.09	Joback Method
cpg	1052.22	J/molxK	1057.55	Joback Method
cpg	1062.69	J/molxK	1091.00	Joback Method
dvisc	0.0004537	Paxs	537.93	Joback Method

dvisc	0.0002484	Paxs	596.66	Joback Method
dvisc	0.0001515	Paxs	655.38	Joback Method
dvisc	0.0001002	Paxs	714.11	Joback Method
dvisc	0.0000706	Paxs	772.84	Joback Method
dvisc	0.0000523	Paxs	831.56	Joback Method
dvisc	0.0000403	Paxs	890.29	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=U380506&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380506&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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