

# Glutaric acid, 8-chlorooctyl 4-bromo-2-methoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C20H28BrClO5/c1-25-18-15-16(21)11-12-17(18)27-20(24)10-8-9-19(23)26-14
<b>InchiKey:</b>	JROSGHXZWPDSKV-UHFFFAOYSA-N
<b>Formula:</b>	C20H28BrClO5
<b>SMILES:</b>	COc1cc(Br)ccc1OC(=O)CCCC(=O)OCCCCCCCCCI
<b>Mol. weight [g/mol]:</b>	463.79

## Physical Properties

Property code	Value	Unit	Source
gf	-359.78	kJ/mol	Joback Method
hf	-853.77	kJ/mol	Joback Method
hfus	57.06	kJ/mol	Joback Method
hvap	95.26	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.656		Crippen Method
mcvol	319.390	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpola	3192.00		NIST Webbook
tb	972.23	K	Joback Method
tc	1192.96	K	Joback Method
tf	622.89	K	Joback Method
vc	1.224	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.90	J/molxK	972.23	Joback Method
cpg	980.35	J/molxK	1009.02	Joback Method
cpg	991.47	J/molxK	1045.81	Joback Method
cpg	1001.28	J/molxK	1082.59	Joback Method
cpg	1009.80	J/molxK	1119.38	Joback Method
cpg	1017.05	J/molxK	1156.17	Joback Method
cpg	1023.03	J/molxK	1192.96	Joback Method
dvisc	0.0001976	Paxs	622.89	Joback Method
dvisc	0.0001233	Paxs	681.11	Joback Method

dvisc	0.0000828	Paxs	739.34	Joback Method
dvisc	0.0000590	Paxs	797.56	Joback Method
dvisc	0.0000440	Paxs	855.78	Joback Method
dvisc	0.0000340	Paxs	914.01	Joback Method
dvisc	0.0000272	Paxs	972.23	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=U393894&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393894&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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