

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

Inchi:	InChI=1S/C28H45BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-22-32-27(30)19-16-20-28(31)
InchiKey:	RKAWWBCITWOERN-UHFFFAOYSA-N
Formula:	C28H45BrO4
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]:	525.56

## Physical Properties

Property code	Value	Unit	Source
gf	-165.86	kJ/mol	Joback Method
hf	-859.46	kJ/mol	Joback Method
hfus	72.79	kJ/mol	Joback Method
hvap	105.61	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.340		Crippen Method
mvol	414.000	ml/mol	McGowan Method
pc	850.48	kPa	Joback Method
rinpol	3656.00		NIST Webbook
rinpol	3656.00		NIST Webbook
tb	1090.44	K	Joback Method
tc	1344.26	K	Joback Method
tf	648.38	K	Joback Method
vc	1.605	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1408.55	J/molxK	1090.44	Joback Method
cpg	1425.23	J/molxK	1132.74	Joback Method
cpg	1440.14	J/molxK	1175.05	Joback Method
cpg	1453.37	J/molxK	1217.35	Joback Method
cpg	1465.03	J/molxK	1259.65	Joback Method
cpg	1475.23	J/molxK	1301.96	Joback Method
cpg	1484.05	J/molxK	1344.26	Joback Method
dvisc	0.0001450	Paxs	648.38	Joback Method

dvisc	0.0000779	Paxs	722.06	Joback Method
dvisc	0.0000469	Paxs	795.73	Joback Method
dvisc	0.0000308	Paxs	869.41	Joback Method
dvisc	0.0000216	Paxs	943.09	Joback Method
dvisc	0.0000159	Paxs	1016.76	Joback Method
dvisc	0.0000123	Paxs	1090.44	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=U377218&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377218&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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