

# Glutaric acid, di(3-iodobenzyl) ester

<b>Inchi:</b>	InChI=1S/C19H18I2O4/c20-16-6-1-4-14(10-16)12-24-18(22)8-3-9-19(23)25-13-15-5-2-7-
<b>InchiKey:</b>	JGCCFSUAYKAGPF-UHFFFAOYSA-N
<b>Formula:</b>	C19H18I2O4
<b>SMILES:</b>	O=C(CCCC(=O)OCc1cccc(I)c1)OCc1cccc(I)c1
<b>Mol. weight [g/mol]:</b>	564.15

## Physical Properties

Property code	Value	Unit	Source
gf	-36.94	kJ/mol	Joback Method
hf	-321.23	kJ/mol	Joback Method
hfus	46.66	kJ/mol	Joback Method
hvap	100.82	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	4.853		Crippen Method
mcvol	297.570	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	3422.00		NIST Webbook
rinpol	3422.00		NIST Webbook
tb	1036.30	K	Joback Method
tc	1300.83	K	Joback Method
tf	642.21	K	Joback Method
vc	1.107	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.42	J/mol×K	1036.30	Joback Method
cpg	807.75	J/mol×K	1080.39	Joback Method
cpg	815.93	J/mol×K	1124.48	Joback Method
cpg	823.05	J/mol×K	1168.57	Joback Method
cpg	829.19	J/mol×K	1212.66	Joback Method
cpg	834.43	J/mol×K	1256.75	Joback Method
cpg	838.87	J/mol×K	1300.83	Joback Method
dvisc	0.0002530	Paxs	642.21	Joback Method

dvisc	0.0001523	Paxs	707.89	Joback Method
dvisc	0.0001000	Paxs	773.57	Joback Method
dvisc	0.0000701	Paxs	839.25	Joback Method
dvisc	0.0000517	Paxs	904.94	Joback Method
dvisc	0.0000398	Paxs	970.62	Joback Method
dvisc	0.0000316	Paxs	1036.30	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=U376993&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376993&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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