

# Isobutyl glucuronide, methyl ester, triacetate

<b>Inchi:</b>	InChI=1S/C17H26O10/c1-8(2)7-23-17-15(26-11(5)20)13(25-10(4)19)12(24-9(3)18)14(27
<b>InchiKey:</b>	CPMQMPQIVULEAS-UHFFFAOYSA-N
<b>Formula:</b>	C17H26O10
<b>SMILES:</b>	COC(=O)C1OC(OCC(C)C)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	390.38

## Physical Properties

Property code	Value	Unit	Source
gf	-1043.37	kJ/mol	Joback Method
hf	-1669.95	kJ/mol	Joback Method
hfus	52.70	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	0.352		Crippen Method
mcvol	281.030	ml/mol	McGowan Method
pc	1466.85	kPa	Joback Method
rinsol	2000.00		NIST Webbook
tb	943.32	K	Joback Method
tc	1159.31	K	Joback Method
tf	594.21	K	Joback Method
vc	1.046	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.52	J/molxK	943.32	Joback Method
cpg	970.67	J/molxK	979.32	Joback Method
cpg	980.75	J/molxK	1015.32	Joback Method
cpg	988.69	J/molxK	1051.31	Joback Method
cpg	994.43	J/molxK	1087.31	Joback Method
cpg	997.91	J/molxK	1123.31	Joback Method
cpg	999.05	J/molxK	1159.31	Joback Method
dvisc	0.0004525	Paxs	594.21	Joback Method
dvisc	0.0002926	Paxs	652.39	Joback Method

dvisc	0.0002032	Paxs	710.58	Joback Method
dvisc	0.0001491	Paxs	768.77	Joback Method
dvisc	0.0001143	Paxs	826.95	Joback Method
dvisc	0.0000908	Paxs	885.13	Joback Method
dvisc	0.0000741	Paxs	943.32	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=R554499&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R554499&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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