

# Ethyl glucuronide, methyl ester, triacetate

<b>Inchi:</b>	InChI=1S/C15H22O10/c1-6-21-15-13(24-9(4)18)11(23-8(3)17)10(22-7(2)16)12(25-15)14
<b>InchiKey:</b>	CWYBDXQVVNLNJG-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O10
<b>SMILES:</b>	CCOC1OC(C(=O)OC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	362.33

## Physical Properties

Property code	Value	Unit	Source
gf	-1057.77	kJ/mol	Joback Method
hf	-1623.39	kJ/mol	Joback Method
hfus	51.04	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	-0.284		Crippen Method
mcvol	252.850	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	898.00	K	Joback Method
tc	1109.52	K	Joback Method
tf	586.67	K	Joback Method
vc	0.940	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.38	J/molxK	898.00	Joback Method
cpg	854.02	J/molxK	933.25	Joback Method
cpg	864.88	J/molxK	968.51	Joback Method
cpg	873.87	J/molxK	1003.76	Joback Method
cpg	880.94	J/molxK	1039.01	Joback Method
cpg	886.01	J/molxK	1074.27	Joback Method
cpg	889.02	J/molxK	1109.52	Joback Method
dvisc	0.0005178	Paxs	586.67	Joback Method

dvisc	0.0003573	Paxs	638.56	Joback Method
dvisc	0.0002607	Paxs	690.45	Joback Method
dvisc	0.0001988	Paxs	742.34	Joback Method
dvisc	0.0001570	Paxs	794.22	Joback Method
dvisc	0.0001277	Paxs	846.11	Joback Method
dvisc	0.0001063	Paxs	898.00	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=R554459&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R554459&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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