

# Isopentyl glucuronide, acetate

<b>Inchi:</b>	InChI=1S/C17H26O10/c1-8(2)6-7-23-17-15(26-11(5)20)13(25-10(4)19)12(24-9(3)18)14(2
<b>InchiKey:</b>	SNRAFAUYYZLVHY-UHFFFAOYSA-N
<b>Formula:</b>	C17H26O10
<b>SMILES:</b>	CC(=O)OC1C(OCCC(C)C)OC(C(=O)O)C(OC(C)=O)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	390.38

## Physical Properties

Property code	Value	Unit	Source
gf	-1075.19	kJ/mol	Joback Method
hf	-1689.96	kJ/mol	Joback Method
hfus	55.60	kJ/mol	Joback Method
hvap	110.05	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	0.654		Crippen Method
mcvol	281.030	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	2010.00		NIST Webbook
tb	1013.08	K	Joback Method
tc	1240.35	K	Joback Method
tf	632.80	K	Joback Method
vc	1.046	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.47	J/molxK	1013.08	Joback Method
cpg	989.36	J/molxK	1050.96	Joback Method
cpg	995.99	J/molxK	1088.84	Joback Method
cpg	1000.30	J/molxK	1126.72	Joback Method
cpg	1002.24	J/molxK	1164.60	Joback Method
cpg	1001.76	J/molxK	1202.48	Joback Method
cpg	998.80	J/molxK	1240.35	Joback Method
dvisc	0.0001795	Paxs	632.80	Joback Method
dvisc	0.0000939	Paxs	696.18	Joback Method

dvisc	0.0000548	Paxs	759.56	Joback Method
dvisc	0.0000347	Paxs	822.94	Joback Method
dvisc	0.0000235	Paxs	886.32	Joback Method
dvisc	0.0000167	Paxs	949.70	Joback Method
dvisc	0.0000124	Paxs	1013.08	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=R554528&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R554528&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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