

# Butyl glucuronide, acetate

<b>Inchi:</b>	InChI=1S/C16H24O10/c1-5-6-7-22-16-14(25-10(4)19)12(24-9(3)18)11(23-8(2)17)13(26-
<b>InchiKey:</b>	GNJHQARMHLGXPB-UHFFFAOYSA-N
<b>Formula:</b>	C16H24O10
<b>SMILES:</b>	CCCCOC1OC(C(=O)O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
<b>Mol. weight [g/mol]:</b>	376.36

## Physical Properties

Property code	Value	Unit	Source
gf	-1081.17	kJ/mol	Joback Method
hf	-1664.04	kJ/mol	Joback Method
hfus	56.53	kJ/mol	Joback Method
hvap	108.22	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	0.408		Crippen Method
mcvol	266.940	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	1953.00		NIST Webbook
tb	990.64	K	Joback Method
tc	1212.86	K	Joback Method
tf	636.53	K	Joback Method
vc	0.997	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.23	J/molxK	990.64	Joback Method
cpg	947.38	J/molxK	1175.83	Joback Method
cpg	946.70	J/molxK	1138.79	Joback Method
cpg	943.79	J/molxK	1101.75	Joback Method
cpg	938.71	J/molxK	1064.71	Joback Method
cpg	931.50	J/molxK	1027.68	Joback Method
cpg	945.78	J/molxK	1212.86	Joback Method
dvisc	0.0000162	Paxs	990.64	Joback Method
dvisc	0.0000214	Paxs	931.62	Joback Method

dvisc	0.0000294	Paxs	872.60	Joback Method
dvisc	0.0000422	Paxs	813.59	Joback Method
dvisc	0.0000643	Paxs	754.57	Joback Method
dvisc	0.0001051	Paxs	695.55	Joback Method
dvisc	0.0001882	Paxs	636.53	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=R554404&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R554404&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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