

Ethyl glucuronide, acetate

Inchi:	InChI=1S/C14H20O10/c1-5-20-14-12(23-8(4)17)10(22-7(3)16)9(21-6(2)15)11(24-14)13(
InchiKey:	ZXPYXBIZQOTOCH-UHFFFAOYSA-N
Formula:	C14H20O10
SMILES:	CCOC1OC(C(=O)O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	348.30

Physical Properties

Property code	Value	Unit	Source
gf	-1098.01	kJ/mol	Joback Method
hf	-1622.76	kJ/mol	Joback Method
hfus	51.35	kJ/mol	Joback Method
hvap	103.76	kJ/mol	Joback Method
log10ws	-0.49		Crippen Method
logp	-0.373		Crippen Method
mvol	238.760	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	944.88	K	Joback Method
tc	1159.44	K	Joback Method
tf	613.99	K	Joback Method
vc	0.884	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.35	J/molxK	944.88	Joback Method
cpg	817.06	J/molxK	980.64	Joback Method
cpg	825.00	J/molxK	1016.40	Joback Method
cpg	831.13	J/molxK	1052.16	Joback Method
cpg	835.38	J/molxK	1087.92	Joback Method
cpg	837.71	J/molxK	1123.68	Joback Method
cpg	838.05	J/molxK	1159.44	Joback Method
dvisc	0.0002455	Paxs	613.99	Joback Method

dvisc	0.0001401	Paxs	669.14	Joback Method
dvisc	0.0000870	Paxs	724.29	Joback Method
dvisc	0.0000578	Paxs	779.43	Joback Method
dvisc	0.0000406	Paxs	834.58	Joback Method
dvisc	0.0000297	Paxs	889.73	Joback Method
dvisc	0.0000226	Paxs	944.88	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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