Methyl(methyl 2,3,4-tri-O-acetyl-beta-d-glucopyranosid)uronate

Other names: Methyl glucuronide, methyl ester, triacetate
Inchi: InChI=1S/C14H20O10/c1-6(15)21-9-10(22-7(2)16)12(23-8(3)17)14(20-5)24-11(9)13(18)1
InchiKey: WQZLHCDEZYULJJ-SSKLVLDBSA-N
Formula: C14H20O10
SMILES: COC(=O)C1OC(OC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 348.30
CAS: 34213-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-1066.19	kJ/mol	Joback Method
hf	-1602.75	kJ/mol	Joback Method
hfus	48.45	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-0.26		Crippen Method
logp	-0.674		Crippen Method
mcvol	238.760	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1842.00		NIST Webbook
tb	875.12	K	Joback Method
tc	1086.11	K	Joback Method
tf	575.40	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.70	J/mol×K	875.12	Joback Method
cpg	796.52	J/mol×K	910.28	Joback Method
cpg	807.65	J/mol×K	945.45	Joback Method
cpg	817.02	J/mol×K	980.61	Joback Method
cpg	824.57	J/mol×K	1015.78	Joback Method
cpg	830.22	J/mol×K	1050.94	Joback Method
cpg	833.91	J/mol×K	1086.11	Joback Method

dvisc	0.0005639	Pa×s	575.40	Joback Method
dvisc	0.0003939	Pa×s	625.35	Joback Method
dvisc	0.0002901	Pa×s	675.31	Joback Method
dvisc	0.0002229	Pa×s	725.26	Joback Method
dvisc	0.0001772	Pa×s	775.21	Joback Method
dvisc	0.0001448	Pa×s	825.17	Joback Method
dvisc	0.0001211	Pa×s	875.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34213348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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