Methyl glucuronide, acetate

Inchi: InChI=1S/C13H18O10/c1-5(14)20-8-9(21-6(2)15)11(22-7(3)16)13(19-4)23-10(8)12(17)18
InchiKey: YAYYBTSPWBBXRC-UHFFFAOYSA-N
Formula: C13H18O10
SMILES: COC1OC(C(=O)O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 334.28

Physical Properties

Property code	Value	Unit	Source
gf	-1106.43	kJ/mol	Joback Method
hf	-1602.12	kJ/mol	Joback Method
hfus	48.76	kJ/mol	Joback Method
hvap	101.54	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	-0.763		Crippen Method
mcvol	224.670	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
tb	922.00	K	Joback Method
tc	1134.12	K	Joback Method
tf	602.72	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.47	J/mol×K	922.00	Joback Method
cpg	782.71	J/mol×K	1098.77	Joback Method
cpg	779.77	J/mol×K	1063.42	Joback Method
cpg	775.01	J/mol×K	1028.06	Joback Method
cpg	768.51	J/mol×K	992.71	Joback Method
cpg	760.31	J/mol×K	957.35	Joback Method
cpg	783.80	J/mol×K	1134.12	Joback Method
dvisc	0.0000267	Pa×s	922.00	Joback Method

dvisc	0.0000350	Pa×s	868.79	Joback Method
dvisc	0.0000476	Pa×s	815.57	Joback Method
dvisc	0.0000675	Pa×s	762.36	Joback Method
dvisc	0.0001009	Pa×s	709.15	Joback Method
dvisc	0.0001611	Pa×s	655.93	Joback Method
dvisc	0.0002793	Pa×s	602.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554602&Units=SI

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