Isopropyl glucuronide, acetate

Inchi: InChI=1S/C15H22O10/c1-6(2)21-15-13(24-9(5)18)11(23-8(4)17)10(22-7(3)16)12(25-15)1
InchiKey: FTQZASLCWAGSEX-UHFFFAOYSA-N
Formula: C15H22O10
SMILES: CC(=O)OC1C(OC(C)C)OC(C(=O)O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 362.33

Physical Properties

Property code	Value	Unit	Source
gf	-1092.03	kJ/mol	Joback Method
hf	-1648.68	kJ/mol	Joback Method
hfus	50.42	kJ/mol	Joback Method
hvap	105.60	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	0.016		Crippen Method
mcvol	252.850	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook
tb	967.32	K	Joback Method
tc	1185.71	K	Joback Method
tf	610.26	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.10	J/mol×K	967.32	Joback Method
cpg	892.78	J/mol×K	1149.31	Joback Method
cpg	891.31	J/mol×K	1112.91	Joback Method
cpg	887.76	J/mol×K	1076.52	Joback Method
cpg	882.16	J/mol×K	1040.12	Joback Method
cpg	874.59	J/mol×K	1003.72	Joback Method
cpg	892.10	J/mol×K	1185.71	Joback Method
dvisc	0.0000174	Pa×s	967.32	Joback Method

dvisc	0.0000234	Pa×s	907.81	Joback Method
dvisc	0.0000326	Pa×s	848.30	Joback Method
dvisc	0.0000478	Pa×s	788.79	Joback Method
dvisc	0.0000748	Pa×s	729.28	Joback Method
dvisc	0.0001264	Pa×s	669.77	Joback Method
dvisc	0.0002369	Pa×s	610.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R554568&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