Isobutyl glucuronide, acetate

Inchi: InChI=1S/C16H24O10/c1-7(2)6-22-16-14(25-10(5)19)12(24-9(4)18)11(23-8(3)17)13(26-1
InchiKey: WFXMDGGIWAVIIY-UHFFFAOYSA-N
Formula: C16H24O10
SMILES: CC(=O)OC1C(OCC(C)C)OC(C(=O)O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 376.36

Physical Properties

Property code	Value	Unit	Source
gf	-1083.61	kJ/mol	Joback Method
hf	-1669.32	kJ/mol	Joback Method
hfus	53.01	kJ/mol	Joback Method
hvap	107.83	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.264		Crippen Method
mcvol	266.940	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	990.20	K	Joback Method
tc	1212.52	K	Joback Method
tf	621.53	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.66	J/mol×K	990.20	Joback Method
cpg	931.89	J/mol×K	1027.25	Joback Method
cpg	939.03	J/mol×K	1064.31	Joback Method
cpg	944.04	J/mol×K	1101.36	Joback Method
cpg	946.86	J/mol×K	1138.41	Joback Method
cpg	947.43	J/mol×K	1175.47	Joback Method
cpg	945.70	J/mol×K	1212.52	Joback Method
dvisc	0.0002065	Pa×s	621.53	Joback Method

dvisc	0.0001091	Pa×s	682.98	Joback Method
dvisc	0.0000640	Pa×s	744.42	Joback Method
dvisc	0.0000408	Pa×s	805.87	Joback Method
dvisc	0.0000277	Pa×s	867.31	Joback Method
dvisc	0.0000198	Pa×s	928.76	Joback Method
dvisc	0.0000147	Pa×s	990.20	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=R554484&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