Glucose, 3,6-diethyl, acetylated

Inchi: InChI=1S/C16H26O9/c1-6-20-8-12-13(22-9(3)17)14(21-7-2)15(23-10(4)18)16(25-12)24-1
InchiKey: CEHRPKUHMLBXOI-QMHWVQJVSA-N
Formula: C16H26O9
SMILES: CCOCC1OC(OC(C)=O)C(OC(C)=O)C(OCC)C1OC(C)=O
Mol. weight [g/mol]: 362.37

Physical Properties

Property code	Value	Unit	Source
gf	-920.43	kJ/mol	Joback Method
hf	-1531.45	kJ/mol	Joback Method
hfus	52.03	kJ/mol	Joback Method
hvap	87.20	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.579		Crippen Method
mcvol	265.370	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	2130.00		NIST Webbook
tb	867.01	K	Joback Method
tc	1071.28	K	Joback Method
tf	548.01	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.91	J/mol×K	867.01	Joback Method
cpg	901.07	J/mol×K	901.05	Joback Method
cpg	914.59	J/mol×K	935.10	Joback Method
cpg	926.39	J/mol×K	969.14	Joback Method
cpg	936.44	J/mol×K	1003.19	Joback Method
cpg	944.66	J/mol×K	1037.23	Joback Method
cpg	951.01	J/mol×K	1071.28	Joback Method
dvisc	0.0005161	Pa×s	548.01	Joback Method
dvisc	0.0003433	Pa×s	601.18	Joback Method

dvisc	0.0002440	Pa×s	654.34	Joback Method
dvisc	0.0001825	Pa×s	707.51	Joback Method
dvisc	0.0001422	Pa×s	760.68	Joback Method
dvisc	0.0001145	Pa×s	813.84	Joback Method
dvisc	0.0000946	Pa×s	867.01	Joback Method

Sources

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=R530220&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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