

glucitol, acetylated

Inchi:	InChI=1S/C18H26O12/c1-9(19)25-7-15(27-11(3)21)17(29-13(5)23)18(30-14(6)24)16(28-
InchiKey:	NJVBTKVPPPOFGAT-UHFFFAOYSA-N
Formula:	C18H26O12
SMILES:	CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]:	434.39

Physical Properties

Property code	Value	Unit	Source
gf	-1312.60	kJ/mol	Joback Method
hf	-1904.77	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	109.05	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	-0.161		Crippen Method
mvol	309.120	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	2062.50		NIST Webbook
rinpol	2062.50		NIST Webbook
tb	1067.22	K	Joback Method
tc	1308.46	K	Joback Method
tf	665.58	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.61	J/molxK	1067.22	Joback Method
cpg	1009.62	J/molxK	1268.25	Joback Method
cpg	1015.04	J/molxK	1228.05	Joback Method
cpg	1017.68	J/molxK	1187.84	Joback Method
cpg	1017.61	J/molxK	1147.63	Joback Method
cpg	1014.89	J/molxK	1107.43	Joback Method
cpg	1001.34	J/molxK	1308.46	Joback Method
dvisc	0.0000110	Paxs	1067.22	Joback Method

dvisc	0.0000145	Paxs	1000.28	Joback Method
dvisc	0.0000198	Paxs	933.34	Joback Method
dvisc	0.0000284	Paxs	866.40	Joback Method
dvisc	0.0000433	Paxs	799.46	Joback Method
dvisc	0.0000714	Paxs	732.52	Joback Method
dvisc	0.0001300	Paxs	665.58	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=R488941&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

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