«beta»-D-Glucopyranoside, 4-(acetyloxy)phenyl, tetraacetate

Other names: Arbutin, pentaacetate
Inchi: InChI=1S/C22H26O12/c1-11(23)28-10-18-19(30-13(3)25)20(31-14(4)26)21(32-15(5)27)2
InchiKey: XGHWMISYPPWNDJ-CUUWFGFTSA-N
Formula: C22H26O12
SMILES: CC(=O)OCC1OC(Oc2ccc(OC(C)=O)cc2)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 482.43
CAS: 14698-56-7

Physical Properties

Property code	Value	Unit	Source
gf	-1129.97	kJ/mol	Joback Method
hf	-1787.61	kJ/mol	Joback Method
hfus	65.61	kJ/mol	Joback Method
hvap	119.40	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	1.074		Crippen Method
mcvol	335.160	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
tb	1166.11	K	Joback Method
tc	1429.21	K	Joback Method
tf	776.66	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.09	J/mol×K	1166.11	Joback Method
cpg	1084.17	J/mol×K	1385.36	Joback Method
cpg	1104.70	J/mol×K	1341.51	Joback Method
cpg	1120.74	J/mol×K	1297.66	Joback Method
cpg	1132.40	J/mol×K	1253.81	Joback Method
cpg	1139.82	J/mol×K	1209.96	Joback Method
cpg	1059.04	J/mol×K	1429.21	Joback Method
dvisc	0.0000304	Pa×s	1166.11	Joback Method

dvisc	0.0000366	Pa×s	1101.20	Joback Method
dvisc	0.0000451	Pa×s	1036.29	Joback Method
dvisc	0.0000572	Pa×s	971.38	Joback Method
dvisc	0.0000751	Pa×s	906.48	Joback Method
dvisc	0.0001028	Pa×s	841.57	Joback Method
dvisc	0.0001482	Pa×s	776.66	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=C14698567&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume