4-Methyl-1,2,3,6-tetraacetylglucoside (A)

Inchi: InChI=1S/C15H22O10/c1-7(16)21-6-11-12(20-5)13(22-8(2)17)14(23-9(3)18)15(25-11)24
InchiKey: RJVRCSFBPSWBNJ-BYYAHTNTSA-N
Formula: C15H22O10
SMILES: COC1C(COC(C)=O)OC(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 362.33

Physical Properties

Property code	Value	Unit	Source
gf	-1057.77	kJ/mol	Joback Method
hf	-1623.39	kJ/mol	Joback Method
hfus	51.04	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-0.68		Crippen Method
logp	-0.284		Crippen Method
mcvol	252.850	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1849.00		NIST Webbook
rinpol	1849.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1852.00		NIST Webbook
tb	898.00	K	Joback Method
tc	1109.52	K	Joback Method
tf	586.67	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.38	J/mol×K	898.00	Joback Method
cpg	854.02	J/mol×K	933.25	Joback Method
cpg	864.88	J/mol×K	968.51	Joback Method
cpg	873.87	J/mol×K	1003.76	Joback Method
cpg	880.94	J/mol×K	1039.01	Joback Method
cpg	886.01	J/mol×K	1074.27	Joback Method

cpg	889.02	J/mol×K	1109.52	Joback Method
dvisc	0.0005178	Pa×s	586.67	Joback Method
dvisc	0.0003573	Pa×s	638.56	Joback Method
dvisc	0.0002607	Pa×s	690.45	Joback Method
dvisc	0.0001988	Pa×s	742.34	Joback Method
dvisc	0.0001570	Pa×s	794.22	Joback Method
dvisc	0.0001277	Pa×s	846.11	Joback Method
dvisc	0.0001063	Pa×s	898.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R117609&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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