

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

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:	RJVRCSEFBPSWBNJ-POTWKZLCSA-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	1830.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	898.00	K	Joback Method
tc	1109.52	K	Joback Method
tf	586.67	K	Joback Method
vc	0.940	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.38	J/molxK	898.00	Joback Method
cpg	854.02	J/molxK	933.25	Joback Method
cpg	864.88	J/molxK	968.51	Joback Method
cpg	873.87	J/molxK	1003.76	Joback Method
cpg	880.94	J/molxK	1039.01	Joback Method
cpg	886.01	J/molxK	1074.27	Joback Method
cpg	889.02	J/molxK	1109.52	Joback Method

dvisc	0.0005178	Paxs	586.67	Joback Method
dvisc	0.0003573	Paxs	638.56	Joback Method
dvisc	0.0002607	Paxs	690.45	Joback Method
dvisc	0.0001988	Paxs	742.34	Joback Method
dvisc	0.0001570	Paxs	794.22	Joback Method
dvisc	0.0001277	Paxs	846.11	Joback Method
dvisc	0.0001063	Paxs	898.00	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=R117614&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

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