

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H22O10/c1-7(16)21-6-11-12(22-8(2)17)13(23-9(3)18)14(20-5)15(25-11)24

BVCQQVDJOODWJR-TZZMIGRFSA-N

C15H22O10

COC1C(OC(C)=O)OC(COC(C)=O)C(OC(C)=O)C1OC(C)=O

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	1851.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1839.00		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

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=R117545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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