

2,3,4,6-Tetra-O-Acetyl-1,5-Anhydro-D-galactitol

Inchi:	InChI=1S/C14H20O9/c1-7(15)19-5-11-13(22-9(3)17)14(23-10(4)18)12(6-20-11)21-8(2)16
InchiKey:	ULWHEXUWXLOVPV-XJFOESAGSA-N
Formula:	C14H20O9
SMILES:	CC(=O)OCC1OCC(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	332.30

Physical Properties

Property code	Value	Unit	Source
hfus	46.19	kJ/mol	Joback Method
logp	-0.257		Crippen Method
mcvol	232.890	ml/mol	McGowan Method
rinpol	1886.52		NIST Webbook
tf	337.09	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.06	J/mol×K	857.37	Joback Method
cpg	765.31	J/mol×K	892.53	Joback Method
cpg	777.05	J/mol×K	927.68	Joback Method
cpg	787.24	J/mol×K	962.84	Joback Method
cpg	795.81	J/mol×K	997.99	Joback Method
cpg	802.73	J/mol×K	1033.15	Joback Method
cpg	807.95	J/mol×K	1068.31	Joback Method
dvisc	0.0006753	Pa×s	557.41	Joback Method
dvisc	0.0004526	Pa×s	607.40	Joback Method
dvisc	0.0003224	Pa×s	657.40	Joback Method
dvisc	0.0002409	Pa×s	707.39	Joback Method
dvisc	0.0001871	Pa×s	757.38	Joback Method
dvisc	0.0001499	Pa×s	807.38	Joback Method
dvisc	0.0001233	Pa×s	857.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R179736&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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