1,5-Anhydro-l-rhamnitol triacetate

Other names: 2,3,4-Tri-O-acetyl-1,5-Anhydro-L-rhamnitol
Inchi: InChI=1S/C12H18O7/c1-6-11(18-8(3)14)12(19-9(4)15)10(5-16-6)17-7(2)13/h6,10-12H,5
InchiKey: QPTFIDGGNPUDEM-DDQZHCRQSA-N
Formula: C12H18O7
SMILES: CC(=O)OC1COC(C)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 274.27

Physical Properties

Property code	Value	Unit	Source
gf	-736.40	kJ/mol	Joback Method
hf	-1164.11	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.200		Crippen Method
mcvol	197.270	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1567.79		NIST Webbook
tb	735.32	K	Joback Method
tc	943.30	K	Joback Method
tf	462.71	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.91	J/mol×K	735.32	Joback Method
cpg	611.64	J/mol×K	769.98	Joback Method
cpg	626.24	J/mol×K	804.65	Joback Method
cpg	639.66	J/mol×K	839.31	Joback Method
cpg	651.88	J/mol×K	873.97	Joback Method
cpg	662.85	J/mol×K	908.64	Joback Method
cpg	672.54	J/mol×K	943.30	Joback Method
dvisc	0.0011531	Pa×s	462.71	Joback Method

dvisc	0.0007606	Pa×s	508.15	Joback Method
dvisc	0.0005372	Pa×s	553.58	Joback Method
dvisc	0.0003999	Pa×s	599.01	Joback Method
dvisc	0.0003104	Pa×s	644.45	Joback Method
dvisc	0.0002491	Pa×s	689.88	Joback Method
dvisc	0.0002054	Pa×s	735.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U129023&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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