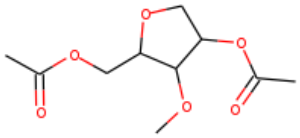
2,5-Di-O-acetyl-1,4-anhydro-3-O-methyl-D-xylitol

Other names: 2,5-O-diAcetyl-1,4-Anhydro-3-O-methyl-D-xylitol.
InChI: InChI=1S/C10H16O6/c1-6(11)14-4-8-10(13-3)9(5-15-8)16-7(2)12/h8-10H,4-5H2,1-3H3
InChI Key: SULWLWFNHXEWRP-UHFFFAOYSA-N
Formula: C10H16O6
SMILES: COC1C(COC(C)=O)OCC1OC(C)=O
Molecular Weight: 232.23



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-604.51	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-983.75	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.47	kJ/mol	Joback Method
$\Delta_{vap} H°$	62.72	kJ/mol	Joback Method
$logP_{oct/wat}$	-0.11		Crippen Method
P_c	2505.01	kPa	Joback Method
T_{boil}	636.09	K	Joback Method
T_c	837.04	K	Joback Method
T_{fus}	398.00	K	Joback Method
V_c	0.62	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	464.89	J/mol×K	636.09	Joback Method
η	0.00	Pa×s	636.09	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H16O6/c1-6(11)14-4-8-10(13-3)9(5-15-8)16-7(2)12/h8-10H,4-5H2,1-3H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).

Latest version available from:
https://www.chemeo.com/cid/86-060-0/2%2C5-Di-O-acetyl-1%2C4-anhydro-3-O-methyl-D-xylitol
Generated by Cheméo on Sun, 21 Jan 2018 12:18:00 +0000.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.