

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.

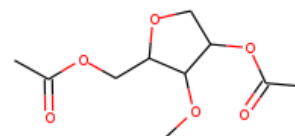
InChI: InChI=1S/C10H16O6/c1-6(11)14-4-8-10(13-3)9(5-15-8)16-7(2)12/h8-10H,4-5H2,1-3H3

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
$\Delta_f G^\circ$	-604.51	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-983.75	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	32.47	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	62.72	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	-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
$C_{p,\text{gas}}$	464.89	J/mol×K	636.09	Joback Method
η	0.00	Paxs	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](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/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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