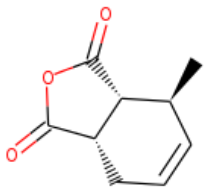
cis,cis-3-Methyl-4-cyclohexene-1,2-dicarboxylic acid anhydride

InChI: InChI=1S/C9H10O3/c1-5-3-2-4-6-7(5)9(11)12-8(6)10/h2-3,5-7H,4H2,1H3/t5-,6-,7+/m1/s1
InChI Key: XPEKVUUBSDFMDR-QYNIQEEDSA-N
Formula: C9H10O3
SMILES: CC1C=CCC2C(=O)OC(=O)C21
Molecular Weight: 166.17
CAS: 35438-82-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-198.95	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-471.93	kJ/mol	Joback Method
$\Delta_f H°_{solid}$	-199.20 ± 1.30	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	18.33	kJ/mol	Joback Method
$\Delta_{vap} H°$	48.96	kJ/mol	Joback Method
$log P_{oct/wat}$	0.90		Crippen Method
P_c	3530.46	kPa	Joback Method
T_{boil}	588.69	K	Joback Method
T_c	838.56	K	Joback Method
T_{fus}	376.04	K	Joback Method
V_c	0.45	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	321.30	J/mol×K	588.69	Joback Method
$\Delta_{sub} H$	49.50 ± 1.00	kJ/mol	325.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H10O3/c1-5-3-2-4-6-7(5)9(11)12-8(6)10/h2-3,5-7H,4H2,1H3/t5-,6-,7+/m1/s1
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f\mathbf{H°_{solid}}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{sub}\mathbf{H}$: Enthalpy of sublimation at a given temperature (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).