

Dimethyl 1,4-cyclohexadiene-1,2-dicarboxylate

InChI: InChI=1S/C10H12O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-4H,5-6H2,1-2H3

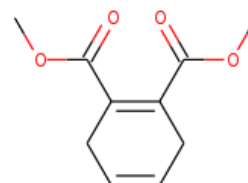
InChI Key: LHDSILFDQOEEGI-UHFFFAOYSA-N

Formula: C10H12O4

SMILES: COC(=O)C1=C(C(=O)OC)CC=CC1

Molecular Weight: 196.20

CAS: 14309-54-7



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-361.70	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-572.05	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	19.66	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	58.81	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	0.979		Crippen Method
P_c	3065.95	kPa	Joback Method
T_{boil}	613.28	K	Joback Method
T_c	830.36	K	Joback Method
T_{fus}	384.96	K	Joback Method
V_c	0.549	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	359.89	J/mol×K	613.28	Joback Method
η	0.0001769	Paxs	613.28	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O4/c1-13-9\(11\)7-5-3-4-6-8\(7\)10\(12\)14-2/h3-4H,5-6H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H12O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-4H,5-6H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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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