Methylaconitic acid, trimethyl ester

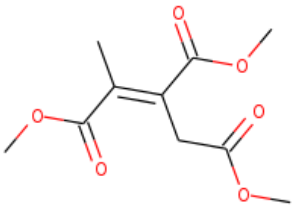
InChI: InChI=1S/C10H14O6/c1-6(9(12)15-3)7(10(13)16-4)5-8(11)14-2/h5H2,1-4H3/b7-6+

InChI Key: ACFSFUFJFGNCSK-VOTSOKGWSA-N

Formula: C10H14O6

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

Molecular Weight: 230.21



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-605.32	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-886.49	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.60	kJ/mol	Joback Method
$\Delta_{vap} H°$	65.44	kJ/mol	Joback Method
$logP_{oct/wat}$	0.21		Crippen Method
P_c	2555.92	kPa	Joback Method
T_{boil}	660.99	K	Joback Method
T_c	859.91	K	Joback Method
T_{fus}	385.94	K	Joback Method
V_c	0.65	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	436.21	J/mol×K	660.99	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H14O6/c1-6(9(12)15-3)7(10(13)16-4)5-8(11)14-2/h5H2,1-4H3/b7-6+

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).