

Dimethylmalonic acid, cis-4-methylcyclohexyl undecyl ester

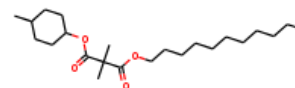
InChI: InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-12-13-18-26-21(24)23(3,4)22(25)27-20-16-14-19(2)15-17-20/h19-20H,5-18H2,1-4H3

InChI Key: VZVVSJRJDZXMHRK-UHFFFAOYSA-N

Formula: C23H42O4

SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1

Molecular Weight: 382.58



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-305.48	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-982.42	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	46.39	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	83.93	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.21		Crippen Method
P_c	1012.30	kPa	Joback Method
T_{boil}	889.87	K	Joback Method
T_c	1093.71	K	Joback Method
T_{fus}	498.85	K	Joback Method
V_c	1.29	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1155.80	J/mol×K	889.87	Joback Method
η	0.00	Paxs	889.87	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-12-13-18-26-21\(24\)23\(3,4\)22\(25\)27-20-16-14-19\(2\)15-17-20/h19-20H,5-18H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H42O4/c1-5-6-7-8-9-10-11-12-13-18-26-21(24)23(3,4)22(25)27-20-16-14-19(2)15-17-20/h19-20H,5-18H2,1-4H3)

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

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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