

Diethylmalonic acid, di(3-methylpent-2-yl) ester

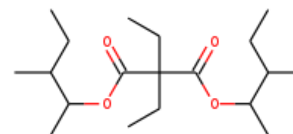
InChI: InChI=1S/C19H36O4/c1-9-13(5)15(7)22-17(20)19(11-3,12-4)18(21)23-16(8)14(6)10-2/h13-16H,9-12H2,1-8H3

InChI Key: DPIIXVCUKNWMOJ-UHFFFAOYSA-N

Formula: C19H36O4

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

Molecular Weight: 328.49



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-365.66	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-954.96	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	29.03	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	73.35	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.75		Crippen Method
P_c	1189.88	kPa	Joback Method
T_{boil}	781.71	K	Joback Method
T_c	972.01	K	Joback Method
T_{fus}	390.63	K	Joback Method
V_c	1.11	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	912.12	J/mol×K	781.71	Joback Method
η	0.00	Paxs	781.71	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H36O4/c1-9-13\(5\)15\(7\)22-17\(20\)19\(11-3,12-4\)18\(21\)23-16\(8\)14\(6\)10-2/h13-16H,9-12H2,1-8H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H36O4/c1-9-13(5)15(7)22-17(20)19(11-3,12-4)18(21)23-16(8)14(6)10-2/h13-16H,9-12H2,1-8H3)

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

Legend

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

η : Dynamic viscosity (Pa×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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