

Diethylmalonic acid, di(2-octyl) ester

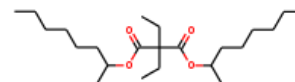
InChI: InChI=1S/C23H44O4/c1-7-11-13-15-17-19(5)26-21(24)23(9-3,10-4)22(25)27-20(6)18-16-14-12-8-2/h19-20H,7-18H2,1-6H3

InChI Key: SSWHDFOWSMCOKF-UHFFFAOYSA-N

Formula: C23H44O4

SMILES: CCCCCC(C)OC(=O)C(CC)(CC)C(=O)OC(C)CCCCC

Molecular Weight: 384.59



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-327.10	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1026.96	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	46.44	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	83.03	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.597		Crippen Method
P_c	918.83	kPa	Joback Method
T_{boil}	874.11	K	Joback Method
T_c	1070.79	K	Joback Method
T_{fus}	465.71	K	Joback Method
V_c	1.349	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1155.68	J/mol×K	874.11	Joback Method
η	0.0000224	Paxs	874.11	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H44O4/c1-7-11-13-15-17-19\(5\)26-21\(24\)23\(9-3,10-4\)22\(25\)27-20\(6\)18-16-14-12-8-2/h19-20H,7-18H2,1-6H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H44O4/c1-7-11-13-15-17-19(5)26-21(24)23(9-3,10-4)22(25)27-20(6)18-16-14-12-8-2/h19-20H,7-18H2,1-6H3)

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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