

Malonic acid, heptyl 3-methylpentyl ester

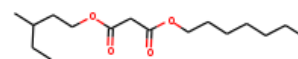
InChI: InChI=1S/C16H30O4/c1-4-6-7-8-9-11-19-15(17)13-16(18)20-12-10-14(3)5-2/h14H,4-13H2,1-3H3

InChI Key: RAUBXYKWOKWCBO-UHFFFAOYSA-N

Formula: C16H30O4

SMILES: CCCCCCOC(=O)CC(=O)OCCC(C)CC

Molecular Weight: 286.41



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-386.44	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-868.45	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.25	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	69.13	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.87		Crippen Method
P_c	1419.71	kPa	Joback Method
T_{boil}	717.62	K	Joback Method
T_c	895.76	K	Joback Method
T_{fus}	399.40	K	Joback Method
V_c	0.97	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	734.08	J/mol×K	717.62	Joback Method
η	0.00	Paxs	717.62	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H30O4/c1-4-6-7-8-9-11-19-15\(17\)13-16\(18\)20-12-10-14\(3\)5-2/h14H,4-13H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H30O4/c1-4-6-7-8-9-11-19-15(17)13-16(18)20-12-10-14(3)5-2/h14H,4-13H2,1-3H3)

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

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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