Glutaric acid, 2-methylhex-3-yl 3-octyl ester

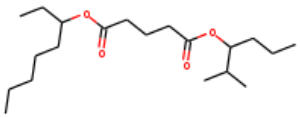
InChI: InChI=1S/C20H38O4/c1-6-9-10-13-17(8-3)23-19(21)14-11-15-20(22)24-18(12-7-2)16(4)5/h16-18H,6-15H2,1-5H3

InChI Key: IPZYSFPRRRZVAB-UHFFFAOYSA-N

Formula: C20H38O4

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

Molecular Weight: 342.51



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-357.64	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-961.57	kJ/mol	Joback Method
$\Delta_{fus} H°$	42.56	kJ/mol	Joback Method
$\Delta_{vap} H°$	77.26	kJ/mol	Joback Method
$logP_{oct/wat}$	5.43		Crippen Method
P_c	1094.99	kPa	Joback Method
T_{boil}	808.26	K	Joback Method
T_c	994.56	K	Joback Method
T_{fus}	414.48	K	Joback Method
V_c	1.19	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	970.62	J/mol×K	808.26	Joback Method
η	0.00	Pa×s	808.26	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H38O4/c1-6-9-10-13-17(8-3)23-19(21)14-11-15-20(22)24-18(12-7-2)16(4)5/h16-18H,6-15H2,1-5H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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