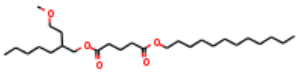
Glutaric acid, dodecyl 2-(2-methoxyethyl)heptyl ester

InChI: InChI=1S/C27H52O5/c1-4-6-8-9-10-11-12-13-14-16-22-31-26(28)19-17-20-27(29)32-24-25(21-23-30-3)18-15-7-5-2/h25H,4-24H2,1-3H3
InChI Key: KWNSUGXRUOSMRS-UHFFFAOYSA-N
Formula: C27H52O5
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCC(CCCCC)CCOC
Molecular Weight: 456.70



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-398.82	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1227.71	kJ/mol	Joback Method
$\Delta_{fus} H°$	68.93	kJ/mol	Joback Method
$\Delta_{vap} H°$	96.03	kJ/mol	Joback Method
$logP_{oct/wat}$	7.40		Crippen Method
P_c	719.91	kPa	Joback Method
T_{boil}	991.72	K	Joback Method
T_c	1229.04	K	Joback Method
T_{fus}	545.60	K	Joback Method
V_c	1.61	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1441.72	J/mol×K	991.72	Joback Method
η	0.00	Pa×s	991.72	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H52O5/c1-4-6-8-9-10-11-12-13-14-16-22-31-26(28)19-17-20-27(29)32-24-25(21-23-30-3)18-15-7-5-2/h25H,4-24H2,1-3H3

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).