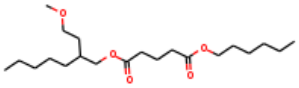
Glutaric acid, hexyl 2-(2-methoxyethyl)heptyl ester

InChI: InChI=1S/C21H40O5/c1-4-6-8-10-16-25-20(22)13-11-14-21(23)26-18-19(15-17-24-3)12-9-7-5-2/h19H,4-18H2,1-3H3
InChI Key: WXRYCEUGCXIFKO-UHFFFAOYSA-N
Formula: C21H40O5
SMILES: CCCCCCOC(=O)CCCC(=O)OCC(CCCCC)CCOC
Molecular Weight: 372.54



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-449.34	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1103.87	kJ/mol	Joback Method
$\Delta_{fus} H°$	53.38	kJ/mol	Joback Method
$\Delta_{vap} H°$	82.67	kJ/mol	Joback Method
$logP_{oct/wat}$	5.06		Crippen Method
P_c	1007.17	kPa	Joback Method
T_{boil}	854.44	K	Joback Method
T_c	1046.32	K	Joback Method
T_{fus}	477.98	K	Joback Method
V_c	1.27	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1062.62	J/mol×K	854.44	Joback Method
η	0.00	Pa×s	854.44	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H40O5/c1-4-6-8-10-16-25-20(22)13-11-14-21(23)26-18-19(15-17-24-3)12-9-7-5-2/h19H,4-18H2,1-3H3

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).