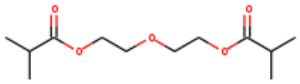
Diethyleneglycol di-isobutyrate

InChI: InChI=1S/C12H22O5/c1-9(2)11(13)16-7-5-15-6-8-17-12(14)10(3)4/h9-10H,5-8H2,1-4H3
InChI Key: MNBUMRSEKNGNCN-UHFFFAOYSA-N
Formula: C12H22O5
SMILES: CC(C)C(=O)OCCOCCOC(=O)C(C)C
Molecular Weight: 246.30
CAS: 76343-97-0



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-527.56	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-923.39	kJ/mol	Joback Method
$\Delta_{fus} H°$	26.55	kJ/mol	Joback Method
$\Delta_{vap} H°$	62.25	kJ/mol	Joback Method
$logP_{oct/wat}$	1.40		Crippen Method
P_c	1925.36	kPa	Joback Method
T_{boil}	648.08	K	Joback Method
T_c	830.65	K	Joback Method
T_{fus}	361.55	K	Joback Method
V_c	0.76	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	544.21	J/mol×K	648.08	Joback Method
η	0.00	Pa×s	648.08	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O5/c1-9(2)11(13)16-7-5-15-6-8-17-12(14)10(3)4/h9-10H,5-8H2,1-4H3
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).