Terephthalic acid, but-3-enyl propyl ester

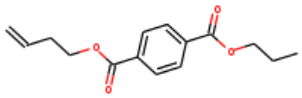
InChI: InChI=1S/C15H18O4/c1-3-5-11-19-15(17)13-8-6-12(7-9-13)14(16)18-10-4-2/h3,6-9H,1,4-5,10-11H2,2H3

InChI Key: CKYKRJSNKQFRSU-UHFFFAOYSA-N

Formula: C15H18O4

SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCC)cc1

Molecular Weight: 262.30



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-201.80	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-492.04	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.55	kJ/mol	Joback Method
$\Delta_{vap} H°$	69.56	kJ/mol	Joback Method
$logP_{oct/wat}$	2.99		Crippen Method
P_c	2051.17	kPa	Joback Method
T_{boil}	723.52	K	Joback Method
T_c	930.26	K	Joback Method
T_{fus}	440.31	K	Joback Method
V_c	0.80	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	569.26	J/mol×K	723.52	Joback Method
η	0.00	Pa×s	723.52	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H18O4/c1-3-5-11-19-15(17)13-8-6-12(7-9-13)14(16)18-10-4-2/h3,6-9H,1,4-5,10-11H2,2H3
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).

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