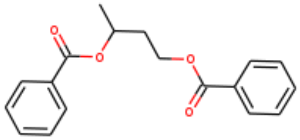
1,3-Butanediol, dibenzoate

InChI: InChI=1S/C18H18O4/c1-14(22-18(20)16-10-6-3-7-11-16)12-13-21-17(19)15-8-4-2-5-9-15/h2-11,14H,12-13H2,1H3
InChI Key: HVWZDMVPWXVEBP-UHFFFAOYSA-N
Formula: C18H18O4
SMILES: CC(CCOC(=O)c1ccccc1)OC(=O)c1ccccc1
Molecular Weight: 298.33



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-144.78	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-436.67	kJ/mol	Joback Method
$\Delta_{fus} H°$	32.51	kJ/mol	Joback Method
$\Delta_{vap} H°$	78.14	kJ/mol	Joback Method
$logP_{oct/wat}$	3.48		Crippen Method
P_c	2096.50	kPa	Joback Method
T_{boil}	816.74	K	Joback Method
T_c	1048.22	K	Joback Method
T_{fus}	474.78	K	Joback Method
V_c	0.87	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	669.97	J/mol×K	816.74	Joback Method
η	0.00	Pa×s	816.74	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C18H18O4/c1-14(22-18(20)16-10-6-3-7-11-16)12-13-21-17(19)15-8-4-2-5-9-15/h2-11,14H,12-13H2,1H3
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).