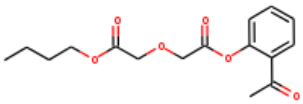
Diglycolic acid, 2-acetylphenyl butyl ester

InChI: InChI=1S/C16H20O6/c1-3-4-9-21-15(18)10-20-11-16(19)22-14-8-6-5-7-13(14)12(2)17/h5-8H,3-4,9-11H2,1-2H3
InChI Key: CTNVLYZEVOPPNW-UHFFFAOYSA-N
Formula: C16H20O6
SMILES: CCCCOC(=O)COCC(=O)Oc1ccccc1C(C)=O
Molecular Weight: 308.33



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-515.14	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-882.91	kJ/mol	Joback Method
$\Delta_{fus} H°$	39.21	kJ/mol	Joback Method
$\Delta_{vap} H°$	81.62	kJ/mol	Joback Method
$logP_{oct/wat}$	2.15		Crippen Method
P_c	1890.36	kPa	Joback Method
T_{boil}	826.01	K	Joback Method
T_c	1034.00	K	Joback Method
T_{fus}	525.50	K	Joback Method
V_c	0.90	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	691.41	J/mol×K	826.01	Joback Method
η	0.00	Pa×s	826.01	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H20O6/c1-3-4-9-21-15(18)10-20-11-16(19)22-14-8-6-5-7-13(14)12(2)17/h5-8H,3-4,9-11H2,1-2H3
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).