

Glutaric acid, butyl 1-phenylethyl ester

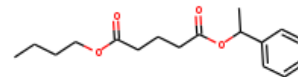
InChI: InChI=1S/C17H24O4/c1-3-4-13-20-16(18)11-8-12-17(19)21-14(2)15-9-6-5-7-10-15/h5-7,9-10,14H,3-4,8,11-13H2,1-2H3

InChI Key: GVPCWSRHGRQQPY-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: CCCCOC(=O)CCCC(=O)OC(C)c1ccccc1

Molecular Weight: 292.37



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-265.61	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-652.56	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	35.88	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	73.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.80		Crippen Method
P_c	1708.95	kPa	Joback Method
T_{boil}	767.18	K	Joback Method
T_c	969.48	K	Joback Method
T_{fus}	437.09	K	Joback Method
V_c	0.92	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	705.62	J/mol×K	767.18	Joback Method
η	0.00	Paxs	767.18	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H24O4/c1-3-4-13-20-16\(18\)11-8-12-17\(19\)21-14\(2\)15-9-6-5-7-10-15/h5-7,9-10,14H,3-4,8,11-13H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H24O4/c1-3-4-13-20-16(18)11-8-12-17(19)21-14(2)15-9-6-5-7-10-15/h5-7,9-10,14H,3-4,8,11-13H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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