

Diethylmalonic acid, butyl 3-nitrophenyl ester

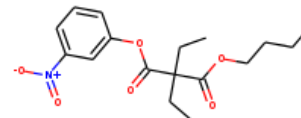
InChI: InChI=1S/C17H23NO6/c1-4-7-11-23-15(19)17(5-2,6-3)16(20)24-1
4-10-8-9-13(12-14)18(21)22/h8-10,12H,4-7,11H2,1-3H3

InChI Key: AOXPJOCZMCUEKS-UHFFFAOYSA-N

Formula: C17H23NO6

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc([N+](=O)[O-])c1

Molecular Weight: 337.37



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-234.41	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-678.26	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	42.96	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	89.98	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.65		Crippen Method
P_c	1720.31	kPa	Joback Method
T_{boil}	921.21	K	Joback Method
T_c	1149.56	K	Joback Method
T_{fus}	610.64	K	Joback Method
V_c	1.00	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	813.12	J/mol×K	921.21	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H23NO6/c1-4-7-11-23-15\(19\)17\(5-2,6-3\)16\(20\)24-14-10-8-9-13\(12-14\)18\(21\)22/h8-10,12H,4-7,11H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H23NO6/c1-4-7-11-23-15(19)17(5-2,6-3)16(20)24-14-10-8-9-13(12-14)18(21)22/h8-10,12H,4-7,11H2,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

$\Delta_f G^\circ$: 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).

$\log P_{oct/wat}$: 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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