

Glutaric acid, 3-nitrobenzyl octyl ester

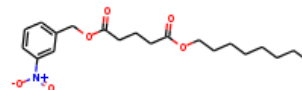
InChI: InChI=1S/C20H29NO6/c1-2-3-4-5-6-7-14-26-19(22)12-9-13-20(23)27-16-17-10-8-11-18(15-17)21(24)25/h8,10-11,15H,2-7,9,12-14,16H2,1H3

InChI Key: GNKRTPWJKOVLFY-UHFFFAOYSA-N

Formula: C20H29NO6

SMILES: CCCCCCOC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1

Molecular Weight: 379.45



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-211.99	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-731.43	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	58.14	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	97.96	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.71		Crippen Method
P_c	1353.63	kPa	Joback Method
T_{boil}	993.08	K	Joback Method
T_c	1218.94	K	Joback Method
T_{fus}	642.03	K	Joback Method
V_c	1.18	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	988.43	J/mol×K	993.08	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H29NO6/c1-2-3-4-5-6-7-14-26-19\(22\)12-9-13-20\(23\)27-16-17-10-8-11-18\(15-17\)21\(24\)25/h8,10-11,15H,2-7,9,12-14,16H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H29NO6/c1-2-3-4-5-6-7-14-26-19(22)12-9-13-20(23)27-16-17-10-8-11-18(15-17)21(24)25/h8,10-11,15H,2-7,9,12-14,16H2,1H3)

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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