

Glutaric acid, 2-isopropylphenyl pentyl ester

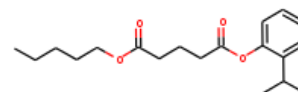
InChI: InChI=1S/C19H28O4/c1-4-5-8-14-22-18(20)12-9-13-19(21)23-17-11-7-6-10-16(17)15(2)3/h6-7,10-11,15H,4-5,8-9,12-14H2,1-3H3

InChI Key: AFDOIPHYAZALQA-UHFFFAOYSA-N

Formula: C19H28O4

SMILES: CCCCCOC(=O)CCCC(=O)Oc1cccc1C(C)C

Molecular Weight: 320.42



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-258.40	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-705.31	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	40.67	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	78.75	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.619		Crippen Method
P_c	1450.14	kPa	Joback Method
T_{boil}	817.92	K	Joback Method
T_c	1019.49	K	Joback Method
T_{fus}	472.15	K	Joback Method
V_c	1.034	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	819.59	J/mol×K	817.92	Joback Method
η	0.0000577	Paxs	817.92	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-4-5-8-14-22-18\(20\)12-9-13-19\(21\)23-17-11-7-6-10-16\(17\)15\(2\)3/h6-7,10-11,15H,4-5,8-9,12-14H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C19H28O4/c1-4-5-8-14-22-18(20)12-9-13-19(21)23-17-11-7-6-10-16(17)15(2)3/h6-7,10-11,15H,4-5,8-9,12-14H2,1-3H3)

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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