

Adipic acid, 2-chloro-5-methylphenyl octyl ester

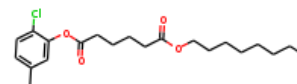
InChI: InChI=1S/C21H31ClO4/c1-3-4-5-6-7-10-15-25-20(23)11-8-9-12-21(24)26-19-16-17(2)13-14-18(19)22/h13-14,16H,3-12,15H2,1-2H3

InChI Key: MOEIBISHZDFKLN-UHFFFAOYSA-N

Formula: C₂₁H₃₁ClO₄

SMILES: CCCCCCOC(=O)CCCC(=O)Oc1cc(C)ccc1Cl

Molecular Weight: 382.92



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-260.68	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-768.52	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	53.18	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	88.64	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.02		Crippen Method
P_c	1207.31	kPa	Joback Method
T_{boil}	906.53	K	Joback Method
T_c	1114.56	K	Joback Method
T_{fus}	552.13	K	Joback Method
V_c	1.20	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	963.52	J/mol×K	906.53	Joback Method
η	0.00	Paxs	906.53	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H31ClO4/c1-3-4-5-6-7-10-15-25-20\(23\)11-8-9-12-21\(24\)26-19-16-17\(2\)13-14-18\(19\)22/h13-14,16H,3-12,15H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C21H31ClO4/c1-3-4-5-6-7-10-15-25-20(23)11-8-9-12-21(24)26-19-16-17(2)13-14-18(19)22/h13-14,16H,3-12,15H2,1-2H3)

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

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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).

Latest version available from:

<https://www.chemeo.com/cid/35-598-0/Adipic%20acid%2C%202-chloro-5-methylphenyl%20octyl%20ester>

Generated by Cheméo on Sat, 18 Sep 2021 01:59:45 +0000.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.