

Valeric acid, 3-methylphenyl ester

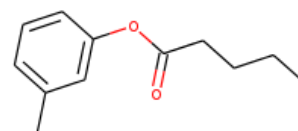
InChI: InChI=1S/C12H16O2/c1-3-4-8-12(13)14-11-7-5-6-10(2)9-11/h5-7,9
H,3-4,8H2,1-2H3

InChI Key: MEKODTPFXNDIKN-UHFFFAOYSA-N

Formula: C12H16O2

SMILES: CCCCC(=O)Oc1cccc(C)c1

Molecular Weight: 192.25



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-80.98	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-310.75	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	23.27	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	54.40	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.09		Crippen Method
P_c	2480.12	kPa	Joback Method
T_{boil}	581.91	K	Joback Method
T_c	788.90	K	Joback Method
T_{fus}	336.10	K	Joback Method
V_c	0.62	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	393.77	J/mol×K	581.91	Joback Method
η	0.00	Paxs	581.91	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16O2/c1-3-4-8-12\(13\)14-11-7-5-6-10\(2\)9-11/h5-7,9H,3-4,8H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16O2/c1-3-4-8-12(13)14-11-7-5-6-10(2)9-11/h5-7,9H,3-4,8H2,1-2H3)

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

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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