Benzoic acid, 4-pentyl-

Other names: 4-Amylbenzoic acid; 4-Pentylbenzoic acid; 4-n-Pentylbenzoic acid; Benzoic acid, p-pentyl-; NSC 169024; p-Amylbenzoic acid; p-Pentylbenzoic acid; p-n-Amylbenzoic acid; p-n-Pentylbenzoic acid; para-Pentylbenzoic acid.

InChI: InChI=1S/C12H16O2/c1-2-3-4-5-10-6-8-11(9-7-10)12(13)14/h6-9H,2-5H2,1H3,(H,13,14)

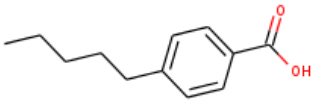
InChI Key: CWYNKKGQJYAHQG-UHFFFAOYSA-N

Formula: C12H16O2

SMILES: CCCCCc1ccc(C(=O)O)cc1

Molecular Weight: 192.25

CAS: 26311-45-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-112.80	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-330.76	kJ/mol	Joback Method
$\Delta_{fus} H°$	26.18	kJ/mol	Joback Method
$\Delta_{sub} H°$	118.20 ± 1.00	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	68.67	kJ/mol	Joback Method
$logP_{oct/wat}$	3.12		Crippen Method
P_c	2773.00	kPa	Joback Method
T_{boil}	651.67	K	Joback Method
T_c	847.74	K	Joback Method
T_{fus}	374.69	K	Joback Method
V_c	0.62	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	424.06	J/mol×K	651.67	Joback Method
η	0.00	Pa×s	651.67	Joback Method

Property	Value	Unit	Temperature (K)	Source
$\Delta_{fus}H$	2.60	kJ/mol	252.0	NIST Webbook
$\Delta_{fus}H$	9.90	kJ/mol	362.0	NIST Webbook
$\Delta_{fus}H$	1.50	kJ/mol	395.0	NIST Webbook
$\Delta_{fus}S$	10.32	J/mol×K	252.0	NIST Webbook
$\Delta_{fus}S$	27.35	J/mol×K	362.0	NIST Webbook
$\Delta_{fus}S$	3.80	J/mol×K	395.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16O2/c1-2-3-4-5-10-6-8-11(9-7-10)12(13)14/h6-9H,2-5H2,1H3,(H,13,14)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H}$: Enthalpy of fusion at a given temperature (kJ/mol).
$\Delta_{sub}\mathbf{H°}$: Enthalpy of sublimation at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\Delta_{fus}\mathbf{S}$: Entropy of fusion at a given temperature (J/mol×K).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).