Benzoyl chloride, 4-(pentyloxy)-

Other names: 4-Pentyloxybenzoyl chloride; 4-n-Amyloxybenzoyl chloride; p-Pentoxybenzoyl chloride; p-Pentyloxybenzoyl chloride.

InChI: InChI=1S/C12H15ClO2/c1-2-3-4-9-15-11-7-5-10(6-8-11)12(13)14/h5-8H,2-4,9H2,1H3

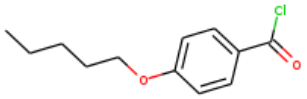
InChI Key: IBQDPNHVFRFCFK-UHFFFAOYSA-N

Formula: C12H15ClO2

SMILES: CCCCCOc1ccc(C(=O)Cl)cc1

Molecular Weight: 226.70

CAS: 36823-84-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-92.91	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-326.49	kJ/mol	Joback Method
$\Delta_{fus} H°$	27.47	kJ/mol	Joback Method
$\Delta_{vap} H°$	58.79	kJ/mol	Joback Method
$logP_{oct/wat}$	3.63		Crippen Method
P_c	2391.19	kPa	Joback Method
T_{boil}	619.34	K	Joback Method
T_c	830.22	K	Joback Method
T_{fus}	366.02	K	Joback Method
V_c	0.67	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	421.33	J/mol×K	619.34	Joback Method
η	0.00	Pa×s	619.34	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H15ClO2/c1-2-3-4-9-15-11-7-5-10(6-8-11)12(13)14/h5-8H,2-4,9H2,1H3
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).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: 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).