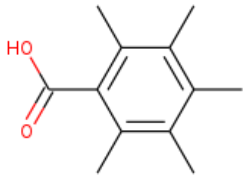
Pentamethylbenzoic acid

Other names: Benzoic acid, pentamethyl-.
InChI: InChI=1S/C12H16O2/c1-6-7(2)9(4)11(12(13)14)10(5)8(6)3/h1-5H3,(H,13,14)
InChI Key: MNLKGWIYXCKWBU-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: Cc1c(C)c(C)c(C(=O)O)c(C)c1C
Molecular Weight: 192.25
CAS: 2243-32-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-151.32	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-422.90 ± 2.90	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	-536.30 ± 2.30	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	24.62	kJ/mol	Joback Method
$\Delta_{sub} H°$	113.40 ± 1.80	kJ/mol	NIST Webbook
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$\Delta_{sub} H°$	113.40 ± 1.80	kJ/mol	NIST Webbook
$\Delta_{vap} H°$	71.32	kJ/mol	Joback Method
$logP_{oct/wat}$	2.93		Crippen Method
P_c	2605.74	kPa	Joback Method
T_{boil}	671.59	K	Joback Method
T_c	871.10	K	Joback Method
T_{fus}	424.77	K	Joback Method
V_c	0.62	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	419.94	J/mol×K	671.59	Joback Method
$C_{p,solid}$	249.90	J/mol×K	298.15	NIST Webbook
η	0.00	Pa×s	671.59	Joback Method
$\Delta_{sub}H$	111.50 ± 1.70	kJ/mol	355.0	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H16O2/c1-6-7(2)9(4)11(12(13)14)10(5)8(6)3/h1-5H3,(H,13,14)
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$C_{p,solid}$: Solid phase heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°$_{gas}$**: Enthalpy of formation at standard conditions (kJ/mol).
Δ_f**H°$_{solid}$**: Solid phase enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{sub}**H°**: Enthalpy of sublimation at standard conditions (kJ/mol).
Δ_{sub}**H**: Enthalpy of sublimation at a given temperature (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P$_{oct/wat}$**: 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 (m^3/kg-mol).

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