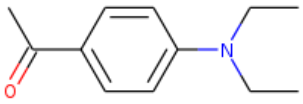
p-Diethylaminoacetophenone

InChI: InChI=1S/C12H17NO/c1-4-13(5-2)12-8-6-11(7-9-12)10(3)14/h6-9H,4-5H2,1-3H3
InChI Key: HMIBQFXWSUBFTG-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCN(CC)c1ccc(C(C)=O)cc1
Molecular Weight: 191.27
CAS: 5520-66-1



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	134.80	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-111.00	kJ/mol	Joback Method
$\Delta_{fus} H°$	25.11	kJ/mol	Joback Method
$\Delta_{vap} H°$	54.03	kJ/mol	Joback Method
$logP_{oct/wat}$	2.74		Crippen Method
P_c	2517.59	kPa	Joback Method
T_{boil}	571.93	K	Joback Method
T_c	778.19	K	Joback Method
T_{fus}	346.34	K	Joback Method
V_c	0.62	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	404.24	J/mol×K	571.93	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17NO/c1-4-13(5-2)12-8-6-11(7-9-12)10(3)14/h6-9H,4-5H2,1-3H3

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

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\mathit{log}P_{oct/wat}}$: 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).

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