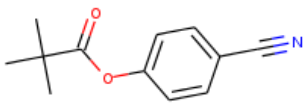
2,2-Dimethylpropanoic acid, 4-cyanophenyl ester

InChI: InChI=1S/C12H13NO2/c1-12(2,3)11(14)15-10-6-4-9(8-13)5-7-10/h4-7H,1-3H3
InChI Key: KVCYRHCBMVONNS-UHFFFAOYSA-N
Formula: C12H13NO2
SMILES: CC(C)(C)C(=O)Oc1ccc(C#N)cc1
Molecular Weight: 203.24



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	55.04	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-154.62	kJ/mol	Joback Method
$\Delta_{fus} H°$	17.37	kJ/mol	Joback Method
$\Delta_{vap} H°$	63.58	kJ/mol	Joback Method
$logP_{oct/wat}$	2.51		Crippen Method
P_c	2465.36	kPa	Joback Method
T_{boil}	680.76	K	Joback Method
T_c	913.60	K	Joback Method
T_{fus}	403.51	K	Joback Method
V_c	0.64	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	423.63	J/mol×K	680.76	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H13NO2/c1-12(2,3)11(14)15-10-6-4-9(8-13)5-7-10/h4-7H,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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