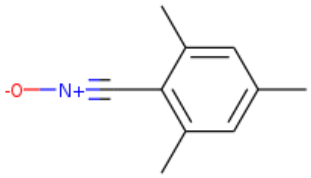
2,4,6-Trimethylbenzonitrile, N-oxide

Other names: 2,4,6-Trimethylbenzonitrile oxide; Benzonitrile, 2,4,6-trimethyl-, N-oxide; Mesitonitrile N-oxide; Mesitonitrile oxide.
InChI: InChI=1S/C10H11NO/c1-7-4-8(2)10(6-11-12)9(3)5-7/h4-5H,1-3H3
InChI Key: ZILPALOUYKHPKI-UHFFFAOYSA-N
Formula: C10H11NO
SMILES: Cc1cc(C)c(C#[N+][O-])c(C)c1
Molecular Weight: 161.20
CAS: 2904-57-6



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-5556.50 ± 2.50	kJ/mol	NIST Webbook
$\Delta_c H°_{solid}$	-5563.10 ± 0.80	kJ/mol	NIST Webbook
$\Delta_f H°_{gas}$	137.00 ± 4.00	kJ/mol	NIST Webbook
$\Delta_f H°_{gas}$	133.40 ± 4.00	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	49.30 ± 3.50	kJ/mol	NIST Webbook
$\Delta_f H°_{solid}$	55.90 ± 1.50	kJ/mol	NIST Webbook
$\Delta_{sub} H°$	87.80 ± 1.80	kJ/mol	NIST Webbook
$\Delta_{sub} H°$	77.50 ± 3.70	kJ/mol	NIST Webbook
IE	8.37	eV	NIST Webbook
IE	8.34	eV	NIST Webbook
IE	8.35 ± 0.02	eV	NIST Webbook
$logP_{oct/wat}$	2.79		Crippen Method
$S°_{solid,1\ bar}$	265.08	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,solid}$	236.10	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook:
http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H11NO/c1-7-4-8(2)10(6-11-12)9(3)5-7/h4-5H,1-3H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\Delta_c H°_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
$C_{p,solid}$: Solid phase heat capacity (J/mol×K).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_f H°_{solid}$: Solid phase enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{sub} H°$: Enthalpy of sublimation at standard conditions (kJ/mol).
IE: Ionization energy (eV).
$logP_{oct/wat}$: Octanol/Water partition coefficient .
$S°_{solid,1\ bar}$: Solid phase molar entropy at standard conditions (J/mol×K).