2,4,6-Trimethylbenzonitrile, N-oxide

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

Physical Properties

Property code	Value	Unit	Source
chs	-5556.50 ± 2.50	kJ/mol	NIST Webbook
chs	-5563.10 ± 0.80	kJ/mol	NIST Webbook
hf	133.40 ± 4.00	kJ/mol	NIST Webbook
hf	137.00 ± 4.00	kJ/mol	NIST Webbook
hfs	49.30 ± 3.50	kJ/mol	NIST Webbook
hfs	55.90 ± 1.50	kJ/mol	NIST Webbook
hsub	77.50 ± 3.70	kJ/mol	NIST Webbook
hsub	87.80 ± 1.80	kJ/mol	NIST Webbook
ie	8.37	eV	NIST Webbook
ie	8.35 ± 0.02	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
log10ws	-6.60		Crippen Method
logp	2.791		Crippen Method
mcvol	135.250	ml/mol	McGowan Method
ss	265.08	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	236.10	J/mol×K	298.15	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2904576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions