4-t-Butylbenzonitrile

Other names:	Benzonitrile, 4-(1,1-dimethylethyl)-
	Benzonitrile, p-tert-butyl-
	p-tert-Butylbenzonitrile
	4-tert-Butyl-benzonitrile
Inchi:	InChI=1S/C11H13N/c1-11(2,3)10-6-4-9(8-12)5-7-10/h4-7H,1-3H3
InchiKey:	IIZURLNRIMKEDL-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	CC(C)(C)c1ccc(C#N)cc1
Mol. weight [g/mol]:	159.23
CAS:	4210-32-6

Physical Properties

Property code	Value	Unit	Source
gf	280.54	kJ/mol	Joback Method
hf	110.82	kJ/mol	Joback Method
hfus	11.99	kJ/mol	Joback Method
hvap	52.20	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	9.11 ± 0.02	eV	NIST Webbook
log10ws	-3.14		Crippen Method
logp	2.856		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
tb	581.59	K	Joback Method
tc	815.92	K	Joback Method
tf	320.08	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.28	J/mol×K	581.59	Joback Method
cpg	351.17	J/mol×K	620.65	Joback Method
cpg	364.04	J/mol×K	659.70	Joback Method

cpg	375.97	J/mol×K	698.76	Joback Method
cpg	387.00	J/mol×K	737.81	Joback Method
cpg	397.23	J/mol×K	776.87	Joback Method
cpg	406.69	J/mol×K	815.92	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4210326&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume