1,2,4,5-Benzenetetracarbonitrile

Other names:	s-Tetracyanobenzene
	Benzene, 1,2,4,5-tetracyano-
	Pyromellitic tetranitrile
	Pyromellitonitrile
	Pyromellitotetranitrile
	1,2,4,5-Benzenetetranitrile
	1,2,4,5-Tetracyanobenzene
	1,2,4,5-Benzentetrakarbonitril
	sym-Tetracyanobenzene
	Pyromellitic acid tetranitrile
	Pyromellitic nitrile
Inchi:	InChI=1S/C10H2N4/c11-3-7-1-8(4-12)10(6-14)2-9(7)5-13/h1-2H
InchiKey:	FAAXSAZENACQBT-UHFFFAOYSA-N
Formula:	C10H2N4
SMILES:	N#Cc1cc(C#N)c(C#N)cc1C#N
Mol. weight [g/mol]:	178.15
CAS:	712-74-3

Physical Properties

Property code	Value	Unit	Source
ea	2.20 ± 0.22	eV	NIST Webbook
gf	649.56	kJ/mol	Joback Method
hf	611.91	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	84.03	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.173		Crippen Method
mcvol	133.520	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
ss	252.70	J/mol×K	NIST Webbook
tb	878.14	K	Joback Method
tc	1136.76	K	Joback Method
tf	526.40	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.23	J/mol×K	1093.65	Joback Method
cpg	301.43	J/mol×K	878.14	Joback Method
cpg	306.16	J/mol×K	921.24	Joback Method
cpg	310.38	J/mol×K	964.35	Joback Method
cpg	314.12	J/mol×K	1007.45	Joback Method
cpg	317.40	J/mol×K	1050.55	Joback Method
cpg	322.62	J/mol×K	1136.76	Joback Method
cps	222.30	J/mol×K	298.15	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C712743&Units=SI

Legend

cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
ea: Electron affinity
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ss: Solid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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