Benzeneacetonitrile, 4-cyano-

Other names:	p-Tolunitrile, «alpha»-cyano-
	«alpha»-Cyano-p-tolunitrile
	p-Cyanobenzylcyanide
	4-Cyanophenylacetonitrile
	«alpha»,4-Dicyanotoluene
Inchi:	InChI=1S/C9H6N2/c10-6-5-8-1-3-9(7-11)4-2-8/h1-4H,5H2
InchiKey:	QILKKAFYAFEWGU-UHFFFAOYSA-N
Formula:	C9H6N2
SMILES:	N#CCc1ccc(C#N)cc1
Mol. weight [g/mol]:	142.16
CAS:	876-31-3

Physical Properties

Property code	Value	Unit	Source
gf	394.04	kJ/mol	Joback Method
hf	325.73	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.624		Crippen Method
mcvol	116.670	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	641.14	K	Joback Method
tc	884.33	K	Joback Method
tf	360.11	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.23	J/mol×K	641.14	Joback Method
cpg	266.88	J/mol×K	681.67	Joback Method
cpg	274.89	J/mol×K	722.20	Joback Method
cpg	282.28	J/mol×K	762.74	Joback Method

cpg	289.09	J/mol×K	803.27	Joback Method
cpg	295.36	J/mol×K	843.80	Joback Method
cpg	301.12	J/mol×K	884.33	Joback Method

Sources

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=C876313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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