Benzeneacetonitrile, «alpha»-methylene-

Other names:	Atroponitrile
	«alpha»-Cyanostyrene
	«alpha»-Phenylacrylonitrile
	Acrylonitrile, 2-phenyl-
	2-Phenylacrylonitrile
	Benzeneacetonitrile, alpha-methylene-
Inchi:	InChI=1S/C9H7N/c1-8(7-10)9-5-3-2-4-6-9/h2-6H,1H2
InchiKey:	RLFXJQPKMZNLMP-UHFFFAOYSA-N
Formula:	C9H7N
SMILES:	C=C(C#N)c1ccccc1
Mol. weight [g/mol]:	129.16
CAS:	495-10-3

Physical Properties

Property code	Value	Unit	Source
gf	349.78	kJ/mol	Joback Method
hf	287.96	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	47.79	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.223		Crippen Method
mcvol	110.990	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	530.64	K	Joback Method
tc	767.86	K	Joback Method
tf	266.88	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.46	J/mol×K	530.64	Joback Method
cpg	236.37	J/mol×K	570.18	Joback Method
cpg	246.46	J/mol×K	609.71	Joback Method

cpg	255.79	J/mol×K	649.25	Joback Method
cpg	264.40	J/mol×K	688.79	Joback Method
cpg	272.34	J/mol×K	728.32	Joback Method
cpg	279.66	J/mol×K	767.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C495103&Units=SI
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

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