Benzeneacetonitrile, «alpha»-methyl-

Other names:	«alpha»-Cyanoethylbenzene
	Hydratroponitrile
	«alpha»-Methylbenzeneacetonitrile
	«alpha»-Methylbenzyl cyanide
	«alpha»-Phenylethyl cyanide
	2-Phenylpropanenitrile
	«alpha»-Phenylpropionitrile
	2-Phenylpropionitrile
	«alpha»-Methylphenylacetonitrile
	2-Phenylpropyl nitrile
	2-phenylpropiononitrile
Inchi:	InChI=1S/C9H9N/c1-8(7-10)9-5-3-2-4-6-9/h2-6,8H,1H3
InchiKey:	NVAOLENBKNECGF-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	CC(C#N)c1ccccc1
Mol. weight [g/mol]:	131.17
CAS:	1823-91-2

Physical Properties

Property code	Value	Unit	Source
gf	268.05	kJ/mol	Joback Method
hf	167.04	kJ/mol	Joback Method
hfus	11.09	kJ/mol	Joback Method
hvap	60.90 ± 0.70	kJ/mol	NIST Webbook
log10ws	-2.52		Crippen Method
logp	2.314		Crippen Method
mcvol	115.290	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1227.00		NIST Webbook
ripol	2038.00		NIST Webbook
tb	533.64	K	Joback Method
tc	766.36	K	Joback Method
tf	267.60	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.19	J/mol×K	727.58	Joback Method
cpg	244.47	J/mol×K	533.64	Joback Method
cpg	256.37	J/mol×K	572.43	Joback Method
cpg	267.46	J/mol×K	611.21	Joback Method
cpg	277.76	J/mol×K	650.00	Joback Method
cpg	287.32	J/mol×K	688.79	Joback Method
cpg	304.39	J/mol×K	766.36	Joback Method
hvapt	60.80 ± 0.70	kJ/mol	301.00	NIST Webbook

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=C1823912&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
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume