Benzeneacetonitrile, 4-methoxy-

Other names:	Acetonitrile, (p-methoxyphenyl)-
	p-Methoxybenzeneacetonitrile
	p-Methoxybenzyl cyanide
	p-Methoxyphenylacetonitrile
	4-Methoxyphenylacetonitrile
	4-Methoxyphenylacetic acid nitrile
	p-Anisylacetonitrile
	Anisylacetonitrile
	NSC 96
Inchi:	InChI=1S/C9H9NO/c1-11-9-4-2-8(3-5-9)6-7-10/h2-5H,6H2,1H3
InchiKey:	PACGLQCRGWFBJH-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	COc1ccc(CC#N)cc1
Mol. weight [g/mol]:	147.17
CAS:	104-47-2

Physical Properties

Property code	Value	Unit	Source
gf	155.86	kJ/mol	Joback Method
hf	28.63	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
ie	8.77 ± 0.05	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	1.761		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1336.00		NIST Webbook
ripol	2305.00		NIST Webbook
tb	559.70	K	NIST Webbook
tc	787.14	K	Joback Method
tf	317.35	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.49	J/mol×K	561.48	Joback Method
cpg	276.53	J/mol×K	599.09	Joback Method
cpg	286.94	J/mol×K	636.70	Joback Method
cpg	296.73	J/mol×K	674.31	Joback Method
cpg	305.90	J/mol×K	711.92	Joback Method
cpg	314.47	J/mol×K	749.53	Joback Method
cpg	322.45	J/mol×K	787.14	Joback Method

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=C104472&Units=SI

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
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