

Benzeneacetonitrile, 3,4-dimethoxy-

Other names:	(3,4-dimethoxyphenyl)acetonitrile 3,4-Dimethoxybenzyl cyanide Acetonitrile, (3,4-dimethoxyphenyl)- Veratryl cyanide homoveratronitrile
Inchi:	InChI=1S/C10H11NO2/c1-12-9-4-3-8(5-6-11)7-10(9)13-2/h3-4,7H,5H2,1-2H3
InchiKey:	ASLSUMISAQDOOB-UHFFFAOYSA-N
Formula:	C10H11NO2
SMILES:	COc1ccc(CC#N)cc1OC
Mol. weight [g/mol]:	177.20
CAS:	93-17-4

Physical Properties

Property code	Value	Unit	Source
gf	49.65	kJ/mol	Joback Method
hf	-135.70	kJ/mol	Joback Method
hfus	24.72	kJ/mol	Heat Capacities and Thermodynamic Properties of (3,4-Dimethoxyphenyl) Acetonitrile (C10H11NO2)
hvap	56.75	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.770		Crippen Method
mcvol	141.120	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
tb	611.76	K	Joback Method
tc	831.48	K	Joback Method
tf	363.37	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.82	J/mol×K	611.76	Joback Method

cpg	344.49	J/mol×K	648.38	Joback Method
cpg	355.55	J/mol×K	685.00	Joback Method
cpg	365.99	J/mol×K	721.62	Joback Method
cpg	375.80	J/mol×K	758.24	Joback Method
cpg	384.97	J/mol×K	794.86	Joback Method
cpg	393.50	J/mol×K	831.48	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.70	K	1.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacities and Thermodynamic Properties of (3,4-Dimethoxyphenyl) Acetone (C ₁₀ H ₁₁ NO ₂):	https://www.doi.org/10.1021/je800203s
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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