(3-Methoxyphenyl)acetonitrile

Other names:	(m-Methoxyphenyl)acetonitrile
	m-Methoxy benzyl cyanide
	Benzeneacetonitrile, 3-methoxy-
Inchi:	InChI=1S/C9H9NO/c1-11-9-4-2-3-8(7-9)5-6-10/h2-4,7H,5H2,1H3
InchiKey:	LXKNAUOWEJWGTE-UHFFFAOYSA-N
Formula:	C9NO
SMILES:	COc1cccc(CC#N)c1
Mol. weight [g/mol]:	138.10
CAS:	19924-43-7

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
log10ws	-2.26		Crippen Method
logp	1.761		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1379.40		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1379.40		NIST Webbook
tb	561.48	K	Joback Method
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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19924437&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/26-857-2/3-Methoxyphenyl-acetonitrile.pdf
Generated by Cheméo on 2024-04-27 09:42:56.726158794 +0000 UTC m=+16500225.646736111.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.