4-METHOXYCINNAMONITRILE

Other names:	2-Propenenitrile, 3-(4-methoxyphenyl)-
	4-Methoxycinnamonitrile cis + trans
	Cinnamonitrile, p-methoxy-
	cis,trans-4-methoxycinnamonitrile
	p-Methoxycinnamonitrile
Inchi:	InChI=1S/C10H9NO/c1-12-10-6-4-9(5-7-10)3-2-8-11/h2-7H,1H3/b3-2-
InchiKey:	CNBCNHHPIBKYBO-NSCUHMNNSA-N
Formula:	C10H9NO
SMILES:	COc1ccc(/C=C/C#N)cc1
Mol. weight [g/mol]:	159.19

Physical Properties

Property code	Value	Unit	Source
hfus	18.20	kJ/mol	Joback Method
hvap	76.15	kJ/mol	Cheméo Relay (1.0)
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-3.18		Cheméo Relay (1.0)
logp	2.232		Crippen Method
mcvol	130.950	ml/mol	McGowan Method
tb	573.27	K	Cheméo Relay (1.0)
tf	337.15 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.31	J/mol×K	588.52	Joback Method
cpg	301.65	J/mol×K	627.10	Joback Method
cpg	312.25	J/mol×K	665.68	Joback Method
cpg	322.15	J/mol×K	704.26	Joback Method
cpg	331.37	J/mol×K	742.84	Joback Method
cpg	339.95	J/mol×K	781.42	Joback Method
cpg	347.93	J/mol×K	820.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.70	K	0.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28446686&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

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

tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/79-769-2/4-METHOXYCINNAMONITRILE.pdf
Generated by Cheméo on 2026-07-21 18:11:14.011377306 +0000 UTC m=+168569.853262682.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.