(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: C9H9NO
SMILES: COc1cccc(CC#N)c1
Mol. weight [g/mol]: 147.18

Physical Properties

Property code	Value	Unit	Source
hf	56.88	kJ/mol	Cheméo Relay (1.0)
hfus	15.41	kJ/mol	Joback Method
hvap	71.98	kJ/mol	Cheméo Relay (1.0)
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-2.19		Cheméo Relay (1.0)
logp	1.761		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
rinpol	1379.40		NIST Webbook
rinpol	1372.00		NIST Webbook
rinpol	1379.40		NIST Webbook
tb	550.53	K	Cheméo Relay (1.0)
tc	758.90	K	Cheméo Relay (1.0)
tf	270.20	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19924437&Units=SI

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

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):

Legend

cpg: Ideal gas heat capacity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point