

m-Methoxybenzotrile

Other names:	m-Methoxybenzotrile 3-Methoxybenzotrile Benzotrile, 3-methoxy- m-Anisonitrile m-Cyanoanisole Benzotrile, m-methoxy-
Inchi:	InChI=1S/C8H7NO/c1-10-8-4-2-3-7(5-8)6-9/h2-5H,1H3
InchiKey:	KLXSUMLEPNAZFK-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	<chem>COc1cccc(C#N)c1</chem>
Mol. weight [g/mol]:	133.15
CAS:	1527-89-5

Physical Properties

Property code	Value	Unit	Source
gf	147.44	kJ/mol	Joback Method
hf	49.27	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	49.23	kJ/mol	Joback Method
ie	9.05 ± 0.04	eV	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
log10ws	-1.94		Crippen Method
logp	1.567		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	538.60	K	Joback Method
tc	768.55	K	Joback Method
tf	306.08	K	Joback Method
vc	0.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.12	J/mol×K	538.60	Joback Method

cpg	232.03	J/mol×K	576.93	Joback Method
cpg	241.36	J/mol×K	615.25	Joback Method
cpg	250.14	J/mol×K	653.58	Joback Method
cpg	258.37	J/mol×K	691.90	Joback Method
cpg	266.06	J/mol×K	730.23	Joback Method
cpg	273.21	J/mol×K	768.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.70	K	1.70	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1527895&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
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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