

3-METHOXYBENZONITRILE

Other names:	m-Methoxybenzonitrile 3-Methoxybenzonitrile Benzonitrile, 3-methoxy- m-Anisonitrile m-Cyanoanisole Benzonitrile, m-methoxy-
Inchi:	InChI=1S/C8H7NO/c1-10-8-4-2-3-7(5-8)6-9/h2-5H,1H3
InchiKey:	KLXSUMLEPNZFK-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	COc1cccc(C#N)c1
Mol. weight [g/mol]:	133.15

Physical Properties

Property code	Value	Unit	Source
af	0.4578		Cheméo Relay (1.0)
gf	147.44	kJ/mol	Joback Method
hf	80.66	kJ/mol	Cheméo Relay (1.0)
hfus	12.82	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Cheméo Relay (1.0)
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.05 ± 0.04	eV	NIST Webbook
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.567		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	518.13	K	Cheméo Relay (1.0)
tc	737.38	K	Cheméo Relay (1.0)
tf	266.45	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1527895&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
mccvol:	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

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