o-Methoxybenzonitrile

Other names:	2-Methoxybenzonitrile
	Benzonitrile, 2-methoxy-
Inchi:	InChI=1S/C8H7NO/c1-10-8-5-3-2-4-7(8)6-9/h2-5H,1H3
InchiKey:	FSTPMFASNVISBU-UHFFFAOYSA-N
Formula:	C8H7NO
SMILES:	COc1ccccc1C#N
Mol. weight [g/mol]:	133.15
CAS:	6609-56-9

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
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	m3/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	408.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6609569&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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume