

(2-Methoxyphenyl)acetonitrile

Other names:	(o-Methoxyphenyl)acetonitrile Benzeneacetonitrile, 2-methoxy-
Inchi:	InChI=1S/C9H9NO/c1-11-9-5-3-2-4-8(9)6-7-10/h2-5H,6H2,1H3
InchiKey:	DWJKILXTMUGXOU-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	COc1ccccc1CC#N
Mol. weight [g/mol]:	147.17
CAS:	7035-03-2

Physical Properties

Property code	Value	Unit	Source
gf	155.86	kJ/mol	Joback Method
hf	28.63	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	51.45	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.761		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	561.48	K	Joback Method
tc	787.14	K	Joback Method
tf	317.35	K	Joback Method
vc	0.475	m3/kmol	Joback Method

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	2.00	NIST Webbook

Sources

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=C7035032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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