

1-Naphthalenecarbonitrile, 2-methoxy-

Other names:	1-Cyano-2-methoxynaphthalene 2-Methoxy-1-naphthalenecarbonitrile 2-Methoxy-1-naphthonitrile 1-Naphthonitrile, 2-methoxy-
Inchi:	InChI=1S/C12H9NO/c1-14-12-7-6-9-4-2-3-5-10(9)11(12)8-13/h2-7H,1H3
InchiKey:	KPIZWRFKCSLGQK-UHFFFAOYSA-N
Formula:	C12H9NO
SMILES:	COc1ccc2ccccc2c1C#N
Mol. weight [g/mol]:	183.21
CAS:	16000-39-8

Physical Properties

Property code	Value	Unit	Source
gf	278.14	kJ/mol	Joback Method
hf	146.31	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	60.43	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.720		Crippen Method
mcvol	143.970	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
tb	654.08	K	Joback Method
tc	896.70	K	Joback Method
tf	396.38	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.83	J/molxK	654.08	Joback Method
cpg	354.36	J/molxK	694.52	Joback Method
cpg	365.05	J/molxK	734.95	Joback Method
cpg	374.96	J/molxK	775.39	Joback Method
cpg	384.13	J/molxK	815.83	Joback Method

cpg	392.62	J/mol×K	856.27	Joback Method
cpg	400.48	J/mol×K	896.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16000398&Units=SI
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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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