Propanenitrile, 3-methoxy-

Other names:	.beta.-methoxypropionitrile
	1-Methoxy-2-cyanoethane
	1-cyano-2-methoxyethane
	2-cyanoethyl methyl ether
	3-Methoxypropannitril
	3-Methoxypropylnitrile
	3-methoxypropanenitrile
	3-methoxypropionitrile
	3-methoxypropiononitrile
	Methyl «beta»-cyanoethyl ether
	NSC 4090
	propionitrile, 3-methoxy-
	«beta»-Methoxypropionitrile
	«beta»-Methyoxypropionitrile
Inchi:	InChI=1S/C4H7NO/c1-6-4-2-3-5/h2,4H2,1H3
InchiKey:	OOWFYDWAMOKVSF-UHFFFAOYSA-N
Formula:	C4H7N
SMILES:	COCCC#N
Mol. weight [g/mol]:	69.11
CAS:	110-67-8

Physical Properties

Property code	Value	Unit	Source
gf	10.98	kJ/mol	Joback Method
hf	-93.23	kJ/mol	Joback Method
hfus	8.81	kJ/mol	Joback Method
hvap	37.39	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.546		Crippen Method
mcvol	74.470	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
rinpol	750.00		NIST Webbook
rinpol	750.00		NIST Webbook
tb	437.70	K	NIST Webbook
tb	436.20	K	NIST Webbook
tc	607.19	K	Joback Method
tf	211.00 ± 0.60	K	NIST Webbook

tf	209.53	K	Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment
tf	210.12 ± 0.20	K	NIST Webbook
tf	210.20 ± 0.10	K	NIST Webbook
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.15	J/mol×K	415.42	Joback Method
cpg	143.44	J/mol×K	447.38	Joback Method
cpg	149.56	J/mol×K	479.34	Joback Method
cpg	155.51	J/mol×K	511.31	Joback Method
cpg	161.26	J/mol×K	543.27	Joback Method
cpg	166.84	J/mol×K	575.23	Joback Method
cpg	172.21	J/mol×K	607.19	Joback Method
cpl	180.60	J/mol×K	300.60	NIST Webbook

Sources

Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment:	https://www.doi.org/10.1016/j.jct.2008.05.012
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=C110678&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
cpl:	Liquid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume