Propanenitrile, 3-(dimethylamino)-

Other names:	3-(Dimethylamino)propanenitrile
	3-(Dimethylamino)propionitrile
	3-(N,N-Dimethylamino)propionitrile
	3-Dimethylaminopropanonitrile
	3-dimethylaminopropiononitrile
	DMAPN
	Dimethylaminopropionitrile
	N,N-(Dimethylamino)-3-propionitrile
	NSC 232
	Propionitrile, 3-(dimethylamino)-
	beta-Dimethylaminopropionitrile
	«beta»-(Dimethylamino)propionitrile
	«beta»-(N-Dimethylamino)propionitrile
	Â«betaÂ»-(Dimethylamino)propionitrile
	Â«betaÂ»-(N-Dimethylamino)propionitrile
Inchi:	InChI=1S/C5H10N2/c1-7(2)5-3-4-6/h3,5H2,1-2H3
InchiKey:	MTPJEFOSTIKRSS-UHFFFAOYSA-N
Formula:	C5H10N2
SMILES:	CN(C)CCC#N
Mol. weight [g/mol]:	98.15
CAS:	1738-25-6

Physical Properties

Property code	Value	Unit	Source
chl	-3440.30 ± 0.50	kJ/mol	NIST Webbook
chl	-3434.00 ± 3.00	kJ/mol	NIST Webbook
gf	235.18	kJ/mol	Joback Method
hf	96.70	kJ/mol	NIST Webbook
hf	90.40	kJ/mol	NIST Webbook
hfl	43.60 ± 0.50	kJ/mol	NIST Webbook
hfus	13.23	kJ/mol	Joback Method
hvap	53.05	kJ/mol	NIST Webbook
log10ws	-0.35		Crippen Method
logp	0.462		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
sl	266.40	J/mol×K	NIST Webbook

tb	446.20	K	NIST Webbook
tc	616.90	K	Joback Method
tf	228.50 ± 0.60	K	NIST Webbook
tf	228.35 ± 0.35	K	NIST Webbook
tf	228.85 ± 0.20	K	NIST Webbook
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.63	J/mol×K	428.32	Joback Method
cpg	189.79	J/mol×K	459.75	Joback Method
cpg	198.52	J/mol×K	491.18	Joback Method
cpg	206.83	J/mol×K	522.61	Joback Method
cpg	214.74	J/mol×K	554.04	Joback Method
cpg	222.25	J/mol×K	585.47	Joback Method
cpg	229.39	J/mol×K	616.90	Joback Method
cpl	212.50	J/mol×K	298.15	NIST Webbook
hvapt	45.90	kJ/mol	387.50	NIST Webbook
hvapt	52.40	kJ/mol	369.00	NIST Webbook
hvapt	44.10 ± 0.20	kJ/mol	303.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.20	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62669e+01
Coeff. B	-5.00354e+03
Coeff. C	-1.66600e+01

Temperature range (K), min.	324.25
Temperature range (K), max.	473.38

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=C1738256&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.