Acetonitrile, (dimethylamino)-

Other names:	(Dimethylamino)acetonitrile
	N-(Cyanomethyl)dimethylamine
	(CH3)2NCH2CN
	Glycinonitrile, N,N-dimethyl-
	2-Dimethylaminoacetonitrile
	UN 2378
Inchi:	InChI=1S/C4H8N2/c1-6(2)4-3-5/h4H2,1-2H3
InchiKey:	PLXBWEPPAAQASG-UHFFFAOYSA-N
Formula:	C4H8N2
SMILES:	CN(C)CC#N
Mol. weight [g/mol]:	84.12
CAS:	926-64-7

Physical Properties

Property code	Value	Unit	Source
affp	884.50	kJ/mol	NIST Webbook
basg	853.70	kJ/mol	NIST Webbook
chl	-2786.38 ± 0.41	kJ/mol	NIST Webbook
gf	226.76	kJ/mol	Joback Method
hf	114.39 ± 0.75	kJ/mol	NIST Webbook
hfl	69.00 ± 0.50	kJ/mol	NIST Webbook
hfus	10.64	kJ/mol	Joback Method
hvap	45.40 ± 0.59	kJ/mol	NIST Webbook
hvap	45.40	kJ/mol	NIST Webbook
ie	8.86	eV	NIST Webbook
ie	8.72 ± 0.05	eV	NIST Webbook
ie	8.72 ± 0.03	eV	NIST Webbook
log10ws	0.07		Crippen Method
logp	0.072		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	714.00		NIST Webbook
rinpol	712.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1243.00		NIST Webbook
ripol	1244.00		NIST Webbook
ripol	1243.00		NIST Webbook

tb	410.70	K	NIST Webbook
tc	595.61	K	Joback Method
tf	232.30	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.64	J/mol×K	563.91	Joback Method
cpg	144.21	J/mol×K	405.44	Joback Method
cpg	152.02	J/mol×K	437.13	Joback Method
cpg	159.46	J/mol×K	468.83	Joback Method
cpg	166.53	J/mol×K	500.52	Joback Method
cpg	173.26	J/mol×K	532.22	Joback Method
cpg	185.71	J/mol×K	595.61	Joback Method
hvapt	45.40 ± 0.60	kJ/mol	292.00	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=C926647&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas 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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume