O-AMINOBENZONITRILE

Other names:	2-Aminobenzonitrile
	2-Cyano-1-aminobenzene
	2-Cyanoaniline
	Anthranilonitrile
	Benzonitrile, o-amino-
	o-Aminobenzonitrile
	o-Cyanoaniline
Inchi:	InChI=1S/C7H6N2/c8-5-6-3-1-2-4-7(6)9/h1-4H,9H2
InchiKey:	HLCPWBZNUKCSBN-UHFFFAOYSA-N
Formula:	C7H6N2
SMILES:	N#Cc1ccccc1N
Mol. weight [g/mol]:	118.14

Physical Properties

Property code	Value	Unit	Source
hf	234.18	kJ/mol	Cheméo Relay (1.0)
hfus	14.24	kJ/mol	Joback Method
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-1.22		Cheméo Relay (1.0)
logp	1.140		Crippen Method
mcvol	97.090	ml/mol	McGowan Method
tb	540.70	K	NIST Webbook
tb	535.50 ± 0.50	K	NIST Webbook
tf	323.50 ± 0.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.89	J/mol×K	565.83	Joback Method
cpg	214.76	J/mol×K	606.97	Joback Method
cpg	222.99	J/mol×K	648.11	Joback Method
cpg	230.59	J/mol×K	689.25	Joback Method
cpg	237.61	J/mol×K	730.39	Joback Method
cpg	244.08	J/mol×K	771.53	Joback Method

cpg	250.02	J/mol×K	812.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.00 ± 2.00	K	1.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1885296&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point