

Benzeneacetonitrile, 4-amino-

Other names:	4-Aminophenylacetonitrile p-Aminobenzyl cyanide p-Aminophenylacetonitrile Benzeneacetonitrile, 4-amino- 4-Aminophenylacetic acid nitrile
Inchi:	InChI=1S/C8H8N2/c9-6-5-7-1-3-8(10)4-2-7/h1-4H,5,10H2
InchiKey:	YCWRFIYBUQBHJI-UHFFFAOYSA-N
Formula:	C8H8N2
SMILES:	N#CCc1ccc(N)cc1
Mol. weight [g/mol]:	132.17

Physical Properties

Property code	Value	Unit	Source
hfus	16.83	kJ/mol	Joback Method
hvap	75.77	kJ/mol	Cheméo Relay (1.0)
ie	8.26 ± 0.04	eV	NIST Webbook
log10ws	-1.34		Cheméo Relay (1.0)
logp	1.335		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
tb	585.20	K	NIST Webbook
tf	318.84	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.50	J/mol×K	588.71	Joback Method
cpg	259.53	J/mol×K	628.98	Joback Method
cpg	268.84	J/mol×K	669.24	Joback Method
cpg	277.48	J/mol×K	709.51	Joback Method
cpg	285.48	J/mol×K	749.78	Joback Method
cpg	292.87	J/mol×K	790.04	Joback Method
cpg	299.69	J/mol×K	830.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.20	K	1.50	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3544250&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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

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