4-Aminobenzyl cyanide

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]:	132.16
CAS:	3544-25-0

Physical Properties

Property code	Value	Unit	Source
gf	318.89	kJ/mol	Joback Method
hf	215.28	kJ/mol	Joback Method
hfus	16.83	kJ/mol	Joback Method
hvap	57.46	kJ/mol	Joback Method
ie	8.26 ± 0.04	eV	NIST Webbook
log10ws	-1.77		Crippen Method
logp	1.335		Crippen Method
mcvol	111.180	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	585.20	K	NIST Webbook
tc	830.31	K	Joback Method
tf	367.11	K	Joback Method
vc	0.430	m3/kmol	Joback Method

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C3544250&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas 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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume