3-Aminophenylacetic acid nitrile

Inchi: InChI=1S/C8H8N2/c9-5-4-7-2-1-3-8(10)6-7/h1-3,6H,4,10H2
InchiKey: YIZRGZCXUWSHLN-UHFFFAOYSA-N
Formula: C8H8N2
SMILES: N#CCc1cccc(N)c1
Mol. weight [g/mol]: 132.16
CAS: 4623-24-9

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	8.31 ± 0.05	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	588.71	K	Joback Method
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

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=C4623249&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume