Anilino radical

Inchi: InChI=1S/C6H6N/c7-6-4-2-1-3-5-6/h1-5,7H
InchiKey: HSMPSHPWCOOUJH-UHFFFAOYSA-N
Formula: C6H6N
SMILES: [NH]c1ccccc1
Mol. weight [g/mol]: 92.12
CAS: 2348-49-4

Physical Properties

Property code	Value	Unit	Source
affp	949.80	kJ/mol	NIST Webbook
basg	917.40	kJ/mol	NIST Webbook
ea	1.70 ± 0.03	eV	NIST Webbook
ea	1.61 ± 0.00	eV	NIST Webbook
ea	1.69 ± 0.09	eV	NIST Webbook
gf	253.82	kJ/mol	Joback Method
hf	178.64	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	37.52	kJ/mol	Joback Method
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	4.12		Crippen Method
logp	1.601		Crippen Method
mcvol	79.470	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	412.83	K	Joback Method
tc	626.79	K	Joback Method
tf	252.83	K	Joback Method
vc	0.289	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.13	J/mol×K	412.83	Joback Method
cpg	144.12	J/mol×K	448.49	Joback Method
cpg	153.32	J/mol×K	484.15	Joback Method

cpg	161.77	J/mol×K	519.81	Joback Method
cpg	169.53	J/mol×K	555.47	Joback Method
cpg	176.66	J/mol×K	591.13	Joback Method
cpg	183.21	J/mol×K	626.79	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=C2348494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
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