2-Amino-4-iodotoluene

Other names: Benzenamine, 5-iodo-2-methyl-
5-iodo-o-toluidine
Inchi: InChI=1S/C7H8IN/c1-5-2-3-6(8)4-7(5)9/h2-4H,9H2,1H3
InchiKey: IOEHXNCBPIBDBZ-UHFFFAOYSA-N
Formula: C7H8IN
SMILES: Cc1ccc(I)cc1N
Mol. weight [g/mol]: 233.05
CAS: 83863-33-6

Physical Properties

Property code	Value	Unit	Source
gf	225.78	kJ/mol	Joback Method
hf	136.44	kJ/mol	Joback Method
hfus	16.75	kJ/mol	Joback Method
hvap	54.79	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.182		Crippen Method
mcvol	121.530	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	561.87	K	Joback Method
tc	826.21	K	Joback Method
tf	361.43	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.57	J/mol×K	561.87	Joback Method
cpg	238.72	J/mol×K	605.93	Joback Method
cpg	248.09	J/mol×K	649.98	Joback Method
cpg	256.74	J/mol×K	694.04	Joback Method
cpg	264.72	J/mol×K	738.10	Joback Method
cpg	272.07	J/mol×K	782.16	Joback Method
cpg	278.85	J/mol×K	826.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C83863336&Units=SI

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
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