4,5-Dimethyl-ortho-phenylenediamine

Other names: 4,5-Dimethyl-o-phenylenediamine
1,2-Benzenediamine, 4,5-dimethyl-
Inchi: InChI=1S/C8H12N2/c1-5-3-7(9)8(10)4-6(5)2/h3-4H,9-10H2,1-2H3
InchiKey: XSZYBMMYQCYIPC-UHFFFAOYSA-N
Formula: C8H12N2
SMILES: Cc1cc(N)c(N)cc1C
Mol. weight [g/mol]: 136.19
CAS: 3171-45-7

Physical Properties

Property code	Value	Unit	Source
gf	232.90	kJ/mol	Joback Method
hf	61.25	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.468		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	569.12	K	Joback Method
tc	805.53	K	Joback Method
tf	410.42	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.41	J/mol×K	569.12	Joback Method
cpg	292.34	J/mol×K	608.52	Joback Method
cpg	303.57	J/mol×K	647.92	Joback Method
cpg	314.13	J/mol×K	687.33	Joback Method
cpg	324.03	J/mol×K	726.73	Joback Method
cpg	333.29	J/mol×K	766.13	Joback Method
cpg	341.94	J/mol×K	805.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3171457&Units=SI
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

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