4,5-Dimethyl-o-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]: 136.20

Physical Properties

Property code	Value	Unit	Source
af	0.5802		Cheméo Relay (1.0)
gf	232.90	kJ/mol	Joback Method
hf	39.50	kJ/mol	Cheméo Relay (1.0)
hfus	19.74	kJ/mol	Joback Method
hvap	73.36	kJ/mol	Cheméo Relay (1.0)
ie	7.21	eV	Cheméo Relay (1.0)
log10ws	-2.12		Cheméo Relay (1.0)
logp	1.468		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	554.28	K	Cheméo Relay (1.0)
tc	785.68	K	Cheméo Relay (1.0)
tf	432.53	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3171457&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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