P-phenylenediamine, 2-tert-butyl-n-methyl

Inchi: InChI=1S/C11H18N2/c1-11(2,3)9-7-8(12)5-6-10(9)13-4/h5-7,13H,12H2,1-4H3
InchiKey: HNFHRZLIFDCAOV-UHFFFAOYSA-N
Formula: C11H18N2
SMILES: CNc1ccc(N)cc1C(C)(C)C
Mol. weight [g/mol]: 178.27

Physical Properties

Property code	Value	Unit	Source
gf	293.57	kJ/mol	Joback Method
hf	21.73	kJ/mol	Joback Method
hfus	20.39	kJ/mol	Joback Method
hvap	59.46	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.608		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	607.19	K	Joback Method
tc	834.12	K	Joback Method
tf	403.53	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.43	J/mol×K	607.19	Joback Method
cpg	432.16	J/mol×K	645.01	Joback Method
cpg	446.83	J/mol×K	682.83	Joback Method
cpg	460.51	J/mol×K	720.65	Joback Method
cpg	473.25	J/mol×K	758.48	Joback Method
cpg	485.11	J/mol×K	796.30	Joback Method
cpg	496.16	J/mol×K	834.12	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=B6008473&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
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