N,N,2,4,6-Pentamethylbenzenamine

Other names: Benzenamine,N,N,2,4,6-pentamethyl-
N,N,2,4,6-Pentamethylaniline
Inchi: InChI=1S/C11H17N/c1-8-6-9(2)11(12(4)5)10(3)7-8/h6-7H,1-5H3
InchiKey: JZBZLRKFJWQZHU-UHFFFAOYSA-N
Formula: C11H17N
SMILES: Cc1cc(C)c(N(C)C)c(C)c1
Mol. weight [g/mol]: 163.26
CAS: 13021-15-3

Physical Properties

Property code	Value	Unit	Source
gf	236.04	kJ/mol	Joback Method
hf	-0.72	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	46.39	kJ/mol	Joback Method
ie	7.24	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	2.678		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
tb	487.20	K	NIST Webbook
tc	708.03	K	Joback Method
tf	310.18	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.51	J/mol×K	505.14	Joback Method
cpg	351.19	J/mol×K	538.96	Joback Method
cpg	366.08	J/mol×K	572.77	Joback Method
cpg	380.21	J/mol×K	606.59	Joback Method
cpg	393.61	J/mol×K	640.40	Joback Method
cpg	406.30	J/mol×K	674.22	Joback Method

cpg	418.30	J/mol×K	708.03	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48067e+01
Coeff. B	-4.18356e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	364.72
Temperature range (K), max.	517.18

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13021153&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume