Benzenamine, 2,6-bis(1-methylethyl)-

Other names: 2,6-Diisopropylaniline
Aniline, 2,6-diisopropyl-
Inchi: InChI=1S/C12H19N/c1-8(2)10-6-5-7-11(9(3)4)12(10)13/h5-9H,13H2,1-4H3
InchiKey: WKBALTUBRZPIPZ-UHFFFAOYSA-N
Formula: C12H19N
SMILES: CC(C)c1cccc(C(C)C)c1N
Mol. weight [g/mol]: 177.29
CAS: 24544-04-5

Physical Properties

Property code	Value	Unit	Source
gf	204.88	kJ/mol	Joback Method
hf	-54.19	kJ/mol	Joback Method
hfus	18.25	kJ/mol	Joback Method
hvap	69.50 ± 0.30	kJ/mol	NIST Webbook
log10ws	-3.48		Crippen Method
logp	3.516		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1404.20		NIST Webbook
rinpol	1404.20		NIST Webbook
tb	530.20	K	NIST Webbook
tc	802.10	K	Joback Method
tf	329.72	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.49	J/mol×K	765.46	Joback Method
cpg	411.42	J/mol×K	582.25	Joback Method
cpg	428.09	J/mol×K	618.89	Joback Method
cpg	443.79	J/mol×K	655.53	Joback Method
cpg	458.57	J/mol×K	692.18	Joback Method

cpg	472.46	J/mol×K	728.82	Joback Method
cpg	497.69	J/mol×K	802.10	Joback Method
hvapt	69.20 ± 0.30	kJ/mol	303.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48798e+01
Coeff. B	-4.53217e+03
Coeff. C	-8.85320e+01
Temperature range (K), min.	399.12
Temperature range (K), max.	562.20

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24544045&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

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

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume