N,N-Di-(n-propyl)benzenamine

Other names:	Aniline, N,N-dipropyl- Benzenamine, N,N-dipropyl- Dipropylamine, N-phenyl- Dipropylaniline N,N-Dipropylaniline N,N-di-n-Propylaniline
Inchi:	InChI=1S/C12H19N/c1-3-10-13(11-4-2)12-8-6-5-7-9-12/h5-9H,3-4,10-11H2,1-2H3
InchiKey:	MMFBQHXDINNBMW-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CCCN(CCC)c1ccccc1
Mol. weight [g/mol]:	177.29
CAS:	2217-07-4

Physical Properties

Property code	Value	Unit	Source
affp	963.00	kJ/mol	NIST Webbook
basg	931.10	kJ/mol	NIST Webbook
gf	273.35	kJ/mol	Joback Method
hf	13.05	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	46.62	kJ/mol	Joback Method
ie	6.96	eV	NIST Webbook
ie	7.15	eV	NIST Webbook
ie	6.93	eV	NIST Webbook
log10ws	-3.05		Crippen Method
logp	3.313		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	513.08	K	Joback Method
tc	709.79	K	Joback Method
tf	283.89	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.18	J/mol×K	513.08	Joback Method
cpg	397.70	J/mol×K	545.86	Joback Method
cpg	414.23	J/mol×K	578.65	Joback Method
cpg	429.83	J/mol×K	611.43	Joback Method
cpg	444.53	J/mol×K	644.22	Joback Method
cpg	458.38	J/mol×K	677.00	Joback Method
cpg	471.42	J/mol×K	709.79	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46578e+01
Coeff. B	-4.35069e+03
Coeff. C	-8.43620e+01
Temperature range (K), min.	387.12
Temperature range (K), max.	549.86

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=C2217074&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

Legend

affp:	Proton affinity
basg:	Gas basicity
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