

N-benzyl-n-methyl aniline

Inchi:	InChI=1S/C14H15N/c1-15(14-10-6-3-7-11-14)12-13-8-4-2-5-9-13/h2-11H,12H2,1H3
InchiKey:	LXZGVFCKZRHKMU-UHFFFAOYSA-N
Formula:	C14H15N
SMILES:	CN(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	197.28
CAS:	614-30-2

Physical Properties

Property code	Value	Unit	Source
gf	402.60	kJ/mol	Joback Method
hf	208.30	kJ/mol	Joback Method
hfus	23.12	kJ/mol	Joback Method
hvap	53.35	kJ/mol	Joback Method
ie	7.40 ± 0.10	eV	NIST Webbook
log10ws	-3.49		Crippen Method
logp	3.323		Crippen Method
mcvol	170.580	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
ripol	1680.80		NIST Webbook
ripol	2430.00		NIST Webbook
ripol	2430.00		NIST Webbook
tb	585.52	K	Joback Method
tc	821.07	K	Joback Method
tf	282.40 ± 0.40	K	NIST Webbook
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.79	J/mol×K	585.52	Joback Method
cpg	426.97	J/mol×K	624.78	Joback Method
cpg	443.75	J/mol×K	664.04	Joback Method
cpg	459.20	J/mol×K	703.29	Joback Method
cpg	473.44	J/mol×K	742.55	Joback Method

cpg	486.53	J/mol×K	781.81	Joback Method
cpg	498.57	J/mol×K	821.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C614302&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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