

N,N-Dimethyl-4-isopropylaniline

Inchi:	InChI=1S/C11H17N/c1-9(2)10-5-7-11(8-6-10)12(3)4/h5-9H,1-4H3
InchiKey:	MJRUTYCVCLZWSR-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CC(C)c1ccc(N(C)C)cc1
Mol. weight [g/mol]:	163.26
CAS:	4139-78-0

Physical Properties

Property code	Value	Unit	Source
gf	252.86	kJ/mol	Joback Method
hf	16.94	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
ie	7.41	eV	NIST Webbook
log10ws	-2.56		Crippen Method
logp	2.876		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	494.74	K	Joback Method
tc	699.79	K	Joback Method
tf	270.14	K	Joback Method
vc	0.555	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.40	J/mol×K	494.74	Joback Method
cpg	351.28	J/mol×K	528.92	Joback Method
cpg	367.21	J/mol×K	563.09	Joback Method
cpg	382.23	J/mol×K	597.27	Joback Method
cpg	396.38	J/mol×K	631.44	Joback Method
cpg	409.70	J/mol×K	665.62	Joback Method
cpg	422.22	J/mol×K	699.79	Joback Method

Sources

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=C4139780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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