

N,N,N'-Trimethyl-1,4-phenylenediamine

Other names:	p-Phenylenediamine, N,N,N'-trimethyl-
Inchi:	InChI=1S/C9H14N2/c1-10-8-4-6-9(7-5-8)11(2)3/h4-7,10H,1-3H3
InchiKey:	AWXUBHMURFEJMY-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	CNc1ccc(N(C)C)cc1
Mol. weight [g/mol]:	150.22
CAS:	5369-34-6

Physical Properties

Property code	Value	Unit	Source
gf	327.85	kJ/mol	Joback Method
hf	116.97	kJ/mol	Joback Method
hfus	20.84	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.794		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	499.59	K	Joback Method
tc	707.32	K	Joback Method
tf	315.26	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.56	J/mol×K	499.59	Joback Method
cpg	308.28	J/mol×K	534.21	Joback Method
cpg	322.14	J/mol×K	568.83	Joback Method
cpg	335.17	J/mol×K	603.45	Joback Method
cpg	347.41	J/mol×K	638.07	Joback Method
cpg	358.90	J/mol×K	672.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5369346&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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