

3-Methyl-2-naphthylamine

Other names:	2-Naphthylamine, 3-methyl- 3-Methyl-2-aminonaphthalene 3-Methyl-2-naphthylamine
Inchi:	InChI=1S/C11H11N/c1-8-6-9-4-2-3-5-10(9)7-11(8)12/h2-7H,12H2,1H3
InchiKey:	BJICIOTXNBTOAJ-UHFFFAOYSA-N
Formula:	C11H11N
SMILES:	Cc1cc2ccccc2cc1N
Mol. weight [g/mol]:	157.22

Physical Properties

Property code	Value	Unit	Source
af	0.5204		Cheméo Relay (1.0)
gf	307.99	kJ/mol	Joback Method
hf	129.32	kJ/mol	Cheméo Relay (1.0)
hfus	19.73	kJ/mol	Joback Method
hvap	77.47	kJ/mol	Cheméo Relay (1.0)
ie	7.35	eV	Cheméo Relay (1.0)
log10ws	-2.75		Cheméo Relay (1.0)
logp	2.730		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	283.73		NIST Webbook
rinpol	283.73		NIST Webbook
tb	584.66	K	Cheméo Relay (1.0)
tc	852.44	K	Cheméo Relay (1.0)
tf	374.42	K	Cheméo Relay (1.0)
vc	0.481	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.96	J/mol×K	579.23	Joback Method
cpg	320.42	J/mol×K	620.06	Joback Method
cpg	332.87	J/mol×K	660.89	Joback Method

cpg	344.39	J/mol×K	701.72	Joback Method
cpg	355.05	J/mol×K	742.55	Joback Method
cpg	364.93	J/mol×K	783.38	Joback Method
cpg	374.11	J/mol×K	824.22	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C10546244&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

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

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