

2-NAPHTHALENAMINE, N-METHYL-

Inchi: InChI=1S/C11H11N/c1-12-11-7-6-9-4-2-3-5-10(9)8-11/h2-8,12H,1H3
InchiKey: IJNQJQRKLLCLMC-UHFFFAOYSA-N
Formula: C11H11N
SMILES: CNc1ccc2ccccc2c1
Mol. weight [g/mol]: 157.22

Physical Properties

Property code	Value	Unit	Source
af	0.4899		Cheméo Relay (1.0)
gf	340.56	kJ/mol	Joback Method
hf	159.46	kJ/mol	Cheméo Relay (1.0)
hfus	20.02	kJ/mol	Joback Method
hvap	74.82	kJ/mol	Cheméo Relay (1.0)
ie	7.00	eV	Cheméo Relay (1.0)
log10ws	-3.16		Cheméo Relay (1.0)
logp	2.881		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	590.20	K	NIST Webbook
tc	852.61	K	Cheméo Relay (1.0)
tf	345.95	K	Cheméo Relay (1.0)
vc	0.479	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.17	J/mol×K	551.89	Joback Method
cpg	312.34	J/mol×K	590.91	Joback Method
cpg	325.44	J/mol×K	629.92	Joback Method
cpg	337.56	J/mol×K	668.94	Joback Method
cpg	348.77	J/mol×K	707.96	Joback Method
cpg	359.15	J/mol×K	746.98	Joback Method
cpg	368.77	J/mol×K	785.99	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	440.70	K	1.60	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216673&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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