

1,8-Naphthalenediamine

Other names:	1,8-Naphthylenediamine 1,8-diaminonaphthalene Naphthalene-1,8-diamine
Inchi:	InChI=1S/C10H10N2/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h1-6H,11-12H2
InchiKey:	YFOOEYJGMMJJLS-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	Nc1cccc2cccc(N)c12
Mol. weight [g/mol]:	158.20
CAS:	479-27-6

Physical Properties

Property code	Value	Unit	Source
affp	944.50	kJ/mol	NIST Webbook
basg	912.10	kJ/mol	NIST Webbook
gf	366.02	kJ/mol	Joback Method
hf	222.51	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
hsub	94.10 ± 0.40	kJ/mol	NIST Webbook
hsub	99.00 ± 0.70	kJ/mol	NIST Webbook
hvap	79.60 ± 0.30	kJ/mol	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.004		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	628.88	K	Joback Method
tc	886.31	K	Joback Method
tf	453.14	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	364.95	J/mol×K	843.40	Joback Method
cpg	313.89	J/mol×K	628.88	Joback Method
cpg	325.88	J/mol×K	671.78	Joback Method
cpg	336.89	J/mol×K	714.69	Joback Method
cpg	347.01	J/mol×K	757.59	Joback Method
cpg	356.34	J/mol×K	800.50	Joback Method
cpg	372.95	J/mol×K	886.31	Joback Method
hfust	16.15	kJ/mol	339.80	NIST Webbook
hsubt	97.60 ± 0.70	kJ/mol	326.00	NIST Webbook
hvapt	97.60	kJ/mol	326.09	Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of the 1,5- and 1,8-diaminonaphthalenes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	478.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C479276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of the 1,5- and 1,8-diaminonaphthalenes and 1,5-Naphthalenediamine and 1,8-Naphthalenediamine in Different Solvents:	https://www.doi.org/10.1016/j.jct.2009.09.009
Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of the 1,5- and 1,8-diaminonaphthalenes:	https://www.doi.org/10.1021/acs.jced.8b01214
Joback Method:	https://www.doi.org/10.1021/je060394v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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