1,5-Naphthalenediamine

Other names: 1,5-Naphthylenediamine
1,5-diaminonaphthalene
NCI-C03021
Inchi: InChI=1S/C10H10N2/c11-9-5-1-3-7-8(9)4-2-6-10(7)12/h1-6H,11-12H2
InchiKey: KQSABULTKYLFEV-UHFFFAOYSA-N
Formula: C10H10N2
SMILES: Nc1cccc2c(N)cccc12
Mol. weight [g/mol]: 158.20
CAS: 2243-62-1

Physical Properties

Property code	Value	Unit	Source
gf	366.02	kJ/mol	Joback Method
hf	222.51	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hsub	122.50 ± 0.90	kJ/mol	NIST Webbook
hsub	120.20 ± 0.70	kJ/mol	NIST Webbook
hvap	64.38	kJ/mol	Joback Method
ie	6.74 ± 0.02	eV	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	462.15 ± 2.00	K	NIST Webbook
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.88	J/mol×K	671.78	Joback Method
cpg	372.95	J/mol×K	886.31	Joback Method
cpg	364.95	J/mol×K	843.40	Joback Method

cpg	356.34	J/mol×K	800.50	Joback Method
cpg	347.01	J/mol×K	757.59	Joback Method
cpg	336.89	J/mol×K	714.69	Joback Method
cpg	313.89	J/mol×K	628.88	Joback Method
hsubt	118.50 ± 0.90	kJ/mol	378.00	NIST Webbook
hvapt	118.50	kJ/mol	378.11	Enthalpies of combustion, vapour pressures, and enthalpies of sublimation of the 1,5- and 1,8-diaminonaphthalenes
psub	5.40e-05	kPa	357.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	6.56e-05	kPa	359.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	7.41e-05	kPa	360.40	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	8.56e-05	kPa	361.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	4.42e-05	kPa	355.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	1.46e-04	kPa	366.40	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	1.81e-04	kPa	368.40	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	2.05e-04	kPa	369.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	2.50e-04	kPa	371.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes

psub	3.83e-05	kPa	354.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	3.50e-05	kPa	353.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	2.72e-05	kPa	351.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	2.42e-05	kPa	350.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	2.21e-05	kPa	349.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	1.75e-05	kPa	347.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	1.39e-05	kPa	345.30	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes
psub	1.05e-04	kPa	363.40	Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes

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=C2243621&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:	https://www.doi.org/10.1016/j.jct.2009.09.009
Solubility Determination of 1,5-Naphthalenediamine and 1,8-Naphthalenediamine in Different Solvents and Mixing Properties of Solutions:	https://www.doi.org/10.1021/acs.jced.8b01214
Vapor Pressures and Phase Transitions of a Series of the Aminonaphthalenes:	https://www.doi.org/10.1021/je060394v

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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume