

5-AMINOACENAPHTHENE

Other names:	5-Acenaphthenamine 5-Acenaphtheneamine 5-Acenaphthylenamine, 1,2-dihydro- 5-Aminoacenaphthene
Inchi:	InChI=1S/C12H11N/c13-11-7-6-9-5-4-8-2-1-3-10(11)12(8)9/h1-3,6-7H,4-5,13H2
InchiKey:	JEUAWMJVEYFVNJ-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	Nc1ccc2c3c(cccc13)CC2
Mol. weight [g/mol]:	169.23

Physical Properties

Property code	Value	Unit	Source
hf	162.14	kJ/mol	Cheméo Relay (1.0)
hfus	21.09	kJ/mol	Joback Method
hvap	82.30	kJ/mol	Cheméo Relay (1.0)
ie	6.97	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	2.521		Crippen Method
mcvol	135.840	ml/mol	McGowan Method
rinpol	310.43		NIST Webbook
tb	616.53	K	Cheméo Relay (1.0)
tc	904.22	K	Cheméo Relay (1.0)
tf	381.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.30	J/mol×K	614.23	Joback Method
cpg	347.32	J/mol×K	655.90	Joback Method
cpg	359.26	J/mol×K	697.56	Joback Method
cpg	370.29	J/mol×K	739.23	Joback Method
cpg	380.53	J/mol×K	780.90	Joback Method
cpg	390.14	J/mol×K	822.56	Joback Method
cpg	399.25	J/mol×K	864.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.00 ± 4.00	K	0.10	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C4657936&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/ci990307I>

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

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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