

1-Aminoanthracene

Other names:	1-Anthramine «alpha»-Aminoanthracene 1-Aminoanthracene 1-Anthracylamine Anthracene, 1-amino- 1-Anthrylamine NSC 60017
Inchi:	InChI=1S/C14H11N/c15-14-7-3-6-12-8-10-4-1-2-5-11(10)9-13(12)14/h1-9H,15H2
InchiKey:	YUENFNPLGJCNRB-UHFFFAOYSA-N
Formula:	C14H11N
SMILES:	Nc1cccc2cc3ccccc3cc12
Mol. weight [g/mol]:	193.25

Physical Properties

Property code	Value	Unit	Source
hf	217.32	kJ/mol	Cheméo Relay (1.0)
hfus	24.51	kJ/mol	Joback Method
hvap	96.10	kJ/mol	Cheméo Relay (1.0)
ie	6.89	eV	Cheméo Relay (1.0)
log10ws	-4.27		Cheméo Relay (1.0)
logp	3.575		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	362.83		NIST Webbook
tb	667.05	K	Cheméo Relay (1.0)
tc	969.24	K	Cheméo Relay (1.0)
tf	412.28	K	Cheméo Relay (1.0)
vc	0.571	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.28	J/mol×K	666.85	Joback Method
cpg	402.87	J/mol×K	710.31	Joback Method

cpg	415.31	J/mol×K	753.77	Joback Method
cpg	426.75	J/mol×K	797.22	Joback Method
cpg	437.35	J/mol×K	840.68	Joback Method
cpg	447.26	J/mol×K	884.14	Joback Method
cpg	456.62	J/mol×K	927.60	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C610491&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

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
mccol:	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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