2-Anthracenamine

Other names:	2-Aminoanthracene
	2-Anthracylamine
	2-Anthramine
	2-Anthrylamine
	Anthracene, 2-amino
	«beta»-Aminoanthracene
	Â«betaÂ»-Aminoanthracene
Inchi:	InChI=1S/C14H11N/c15-14-6-5-12-7-10-3-1-2-4-11(10)8-13(12)9-14/h1-9H,15H2
InchiKey:	YCSBALJAGZKWFF-UHFFFAOYSA-N
Formula:	C14H11N
SMILES:	Nc1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]:	193.24
CAS:	613-13-8

Physical Properties

Property code	Value	Unit	Source
gf	439.90	kJ/mol	Joback Method
hf	297.23	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	64.28	kJ/mol	Joback Method
log10ws	-5.17		Estimated Solubility Method
log10ws	-5.17		Aqueous Solubility Prediction Method
logp	3.575		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	367.45		NIST Webbook
rinpol	367.10		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	367.10		NIST Webbook
rinpol	365.89		NIST Webbook
rinpol	366.52		NIST Webbook
tb	666.85	K	Joback Method
tc	927.60	K	Joback Method
tf	510.08	K	Aqueous Solubility Prediction Method
vc	0.585	m3/kmol	Joback Method

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C613138&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: 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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