1-Aminopyrene

Other names:	1-Pyrenamine
	3-Aminopyrene
	Pyrene, amino-
	aminopyrene
	pyren-1-ylamine
Inchi:	InChI=1S/C16H11N/c17-14-9-7-12-5-4-10-2-1-3-11-6-8-13(14)16(12)15(10)11/h1-9H,17H
InchiKey:	YZVWKHVRBDQPMQ-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	Nc1ccc2ccc3cccc4ccc1c2c34
Mol. weight [g/mol]:	217.27
CAS:	1606-67-3

Physical Properties

Property code	Value	Unit	Source
gf	548.00	kJ/mol	Joback Method
hf	390.09	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	70.40	kJ/mol	Joback Method
ie	6.80 ± 0.10	eV	NIST Webbook
log10ws	-0.61		Aqueous Solubility Prediction Method
logp	4.166		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	415.39		NIST Webbook
rinpol	411.20		NIST Webbook
tb	728.87	K	Joback Method
tc	990.34	K	Joback Method
tf	389.82	K	Aqueous Solubility Prediction Method
tf	455.00 ± 3.00	K	NIST Webbook
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.67	J/mol×K	728.87	Joback Method
cpg	452.92	J/mol×K	772.45	Joback Method
cpg	464.34	J/mol×K	816.03	Joback Method
cpg	475.16	J/mol×K	859.60	Joback Method
cpg	485.60	J/mol×K	903.18	Joback Method
cpg	495.86	J/mol×K	946.76	Joback Method
cpg	506.18	J/mol×K	990.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1606673&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

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
ie: Ionization energy
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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