4-Pyrenamine

Other names: 4-Aminopyrene
Inchi: InChI=1S/C16H11N/c17-14-9-12-5-1-3-10-7-8-11-4-2-6-13(14)16(11)15(10)12/h1-9H,17H
InchiKey: AYBSKADMMKVOIV-UHFFFAOYSA-N
Formula: C16H11N
SMILES: Nc1cc2cccc3ccc4cccc1c4c32
Mol. weight [g/mol]: 217.27
CAS: 17075-03-5

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
log10ws	-5.93		Crippen Method
logp	4.166		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	412.31		NIST Webbook
tb	728.87	K	Joback Method
tc	990.34	K	Joback Method
tf	521.70	K	Joback Method
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=C17075035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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