

2-Pyrenamine

Other names:	2-Aminopyrene
Inchi:	InChI=1S/C16H11N/c17-14-8-12-6-4-10-2-1-3-11-5-7-13(9-14)16(12)15(10)11/h1-9H,17H
InchiKey:	MFUFBSLEAGDECJ-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	Nc1cc2ccc3cccc4ccc(c1)c2c34
Mol. weight [g/mol]:	217.27
CAS:	1732-23-6

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	7.40 ± 0.10	eV	NIST Webbook
log10ws	-5.93		Crippen Method
logp	4.166		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	413.83		NIST Webbook
rinpol	413.83		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

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1732236&Units=SI

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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