9,10-Phenanthrenediamine

Inchi: InChI=1S/C14H12N2/c15-13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14(13)16/h1-8H,15-16H2
InchiKey: VPRFQZSTJXHBHL-UHFFFAOYSA-N
Formula: C14H12N2
SMILES: Nc1c(N)c2ccccc2c2ccccc12
Mol. weight [g/mol]: 208.26
CAS: 53348-04-2

Physical Properties

Property code	Value	Unit	Source
gf	496.72	kJ/mol	Joback Method
hf	319.55	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	75.58	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.157		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	744.36	K	Joback Method
tc	1009.99	K	Joback Method
tf	543.44	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.65	J/mol×K	744.36	Joback Method
cpg	455.13	J/mol×K	788.63	Joback Method
cpg	466.67	J/mol×K	832.90	Joback Method
cpg	477.41	J/mol×K	877.17	Joback Method
cpg	487.52	J/mol×K	921.44	Joback Method
cpg	497.13	J/mol×K	965.72	Joback Method
cpg	506.40	J/mol×K	1009.99	Joback Method

Sources

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=C53348042&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume