Phenanthrene, 4-amino

Inchi: InChI=1S/C14H11N/c15-13-7-3-5-11-9-8-10-4-1-2-6-12(10)14(11)13/h1-9H,15H2
InchiKey: AFPNTTFBCMSLLO-UHFFFAOYSA-N
Formula: C14H11N
SMILES: Nc1cccc2ccc3ccccc3c12
Mol. weight [g/mol]: 193.24

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	-4.71		Crippen Method
logp	3.575		Crippen Method
mcvol	155.420	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	353.97		NIST Webbook
rinpol	353.97		NIST Webbook
tb	666.85	K	Joback Method
tc	927.60	K	Joback Method
tf	447.66	K	Joback 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

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=R21671&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume