Benzo[c]phenanthrene, 4-amino

Inchi: InChI=1S/C18H13N/c19-17-7-3-6-16-15(17)11-10-13-9-8-12-4-1-2-5-14(12)18(13)16/h1-
InchiKey: LMQPVUDQAMCUKA-UHFFFAOYSA-N
Formula: C18H13N
SMILES: Nc1cccc2c1ccc1ccc3ccccc3c12
Mol. weight [g/mol]: 243.30

Physical Properties

Property code	Value	Unit	Source
gf	570.60	kJ/mol	Joback Method
hf	394.27	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	4.728		Crippen Method
mcvol	192.320	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	451.51		NIST Webbook
tb	782.33	K	Joback Method
tc	1050.06	K	Joback Method
tf	537.96	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.87	J/mol×K	782.33	Joback Method
cpg	537.53	J/mol×K	826.95	Joback Method
cpg	550.29	J/mol×K	871.57	Joback Method
cpg	562.36	J/mol×K	916.19	Joback Method
cpg	573.96	J/mol×K	960.81	Joback Method
cpg	585.32	J/mol×K	1005.44	Joback Method
cpg	596.64	J/mol×K	1050.06	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=R21407&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
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