9-Aminoanthracene

Inchi: InChI=1S/C14H11N/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H,15H2
InchiKey: LHNICELDCMPPDE-UHFFFAOYSA-N
Formula: C14H11N
SMILES: Nc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]: 193.24
CAS: 779-03-3

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	363.91		NIST Webbook
rinpol	363.91		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:	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=C779033&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