Benzo[a]pyrene, 7-amino

Inchi: InChI=1S/C20H13N/c21-18-11-14-10-13-4-1-2-6-15(13)16-9-8-12-5-3-7-17(18)19(12)20(
InchiKey: BJHPDTFXCVOKGZ-UHFFFAOYSA-N
Formula: C20H13N
SMILES: Nc1cc2cc3ccccc3c3ccc4cccc1c4c23
Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
gf	678.70	kJ/mol	Joback Method
hf	487.13	kJ/mol	Joback Method
hfus	36.29	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	5.319		Crippen Method
mcvol	205.340	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	511.98		NIST Webbook
tb	844.35	K	Joback Method
tc	1111.66	K	Joback Method
tf	612.00	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.81	J/mol×K	844.35	Joback Method
cpg	588.94	J/mol×K	888.90	Joback Method
cpg	601.78	J/mol×K	933.45	Joback Method
cpg	614.61	J/mol×K	978.00	Joback Method
cpg	627.74	J/mol×K	1022.55	Joback Method
cpg	641.43	J/mol×K	1067.11	Joback Method
cpg	656.00	J/mol×K	1111.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21158&Units=SI
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

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