Benz(a)anthracene, 7-nitro-

Other names: 7-Nitro benz(a)anthracene
Inchi: InChI=1S/C18H11NO2/c20-19(21)18-15-8-4-2-6-13(15)11-17-14-7-3-1-5-12(14)9-10-16(
InchiKey: KOPVBVBUIYTJBG-UHFFFAOYSA-N
Formula: C18H11NO2
SMILES: O=[N+]([O-])c1c2ccccc2cc2c1ccc1ccccc12
Mol. weight [g/mol]: 273.29
CAS: 20268-51-3

Physical Properties

Property code	Value	Unit	Source
gf	539.70	kJ/mol	Joback Method
hf	349.72	kJ/mol	Joback Method
hfus	37.67	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	5.054		Crippen Method
mcvol	199.760	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
rinpol	448.88		NIST Webbook
rinpol	448.88		NIST Webbook
tb	861.64	K	Joback Method
tc	1141.16	K	Joback Method
tf	598.31	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.44	J/mol×K	861.64	Joback Method
cpg	570.99	J/mol×K	908.23	Joback Method
cpg	582.94	J/mol×K	954.81	Joback Method
cpg	594.55	J/mol×K	1001.40	Joback Method
cpg	606.06	J/mol×K	1047.99	Joback Method
cpg	617.73	J/mol×K	1094.58	Joback Method

cpg	629.81	J/mol×K	1141.16	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=C20268513&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