

6-Nitrobenzo(a)pyrene

Other names:	Benzo(a)pyrene, 6-nitro- 6-Nitrobenz(a)pyrene
Inchi:	InChI=1S/C20H11NO2/c22-21(23)20-16-7-2-1-6-14(16)15-10-8-12-4-3-5-13-9-11-17(20)
InchiKey:	NMMAFY SZGOFZCM-UHFFFAOYSA-N
Formula:	C20H11NO2
SMILES:	O=[N+](O-)c1c2ccccc2c2ccc3cccc4ccc1c2c43
Mol. weight [g/mol]:	297.31
CAS:	63041-90-7

Physical Properties

Property code	Value	Unit	Source
gf	647.80	kJ/mol	Joback Method
hf	442.58	kJ/mol	Joback Method
hfus	42.46	kJ/mol	Joback Method
hvap	87.55	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	5.645		Crippen Method
mcvol	212.780	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
rinpola	501.71		NIST Webbook
rinpola	501.46		NIST Webbook
rinpola	490.90		NIST Webbook
rinpola	501.46		NIST Webbook
rinpola	490.90		NIST Webbook
tb	923.66	K	Joback Method
tc	1201.98	K	Joback Method
tf	672.35	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.64	J/molxK	923.66	Joback Method
cpg	622.75	J/molxK	970.05	Joback Method

cpg	636.06	J/mol×K	1016.43	Joback Method
cpg	649.93	J/mol×K	1062.82	Joback Method
cpg	664.67	J/mol×K	1109.21	Joback Method
cpg	680.61	J/mol×K	1155.59	Joback Method
cpg	698.10	J/mol×K	1201.98	Joback Method
hfust	30.20	kJ/mol	528.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63041907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hfust:	Enthalpy of fusion at a given temperature
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

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