3-Nitrobenzanthrone

Inchi: InChI=1S/C17H9NO3/c19-17-12-5-2-1-4-10(12)11-8-9-15(18(20)21)13-6-3-7-14(17)16(1
InchiKey: QAJOWHGESRCVLY-UHFFFAOYSA-N
Formula: C17H9NO3
SMILES: O=C1c2ccccc2-c2ccc([N+](=O)[O-])c3cccc1c23
Mol. weight [g/mol]: 275.26

Physical Properties

Property code	Value	Unit	Source
gf	390.83	kJ/mol	Joback Method
hf	181.04	kJ/mol	Joback Method
hfus	35.47	kJ/mol	Joback Method
hvap	82.99	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	3.959		Crippen Method
mcvol	191.540	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	490.00		NIST Webbook
tb	903.15	K	Joback Method
tc	1186.99	K	Joback Method
tf	658.02	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.88	J/mol×K	903.15	Joback Method
cpg	559.60	J/mol×K	950.46	Joback Method
cpg	570.74	J/mol×K	997.76	Joback Method
cpg	581.51	J/mol×K	1045.07	Joback Method
cpg	592.11	J/mol×K	1092.38	Joback Method
cpg	602.74	J/mol×K	1139.68	Joback Method
cpg	613.59	J/mol×K	1186.99	Joback Method

Sources

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=R565241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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