1-Amino-6-nitropyrene

Inchi: InChI=1S/C16H10N2O2/c17-13-7-3-9-2-6-12-14(18(19)20)8-4-10-1-5-11(13)15(9)16(10)
InchiKey: LEMZVQDZDPOLAQ-UHFFFAOYSA-N
Formula: C16H10N2O2
SMILES: Nc1ccc2ccc3c([N+](=O)[O-])ccc4ccc1c2c43
Mol. weight [g/mol]: 262.26

Physical Properties

Property code	Value	Unit	Source
gf	573.92	kJ/mol	Joback Method
hf	367.86	kJ/mol	Joback Method
hfus	40.27	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.074		Crippen Method
mcvol	185.860	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
rinpol	3229.00		NIST Webbook
rinpol	3229.00		NIST Webbook
tb	885.69	K	Joback Method
tc	1162.60	K	Joback Method
tf	677.83	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.08	J/mol×K	885.69	Joback Method
cpg	535.30	J/mol×K	931.84	Joback Method
cpg	546.38	J/mol×K	977.99	Joback Method
cpg	557.58	J/mol×K	1024.15	Joback Method
cpg	569.17	J/mol×K	1070.30	Joback Method
cpg	581.38	J/mol×K	1116.45	Joback Method
cpg	594.49	J/mol×K	1162.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R389270&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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