4-Nitrophenanthrene

Other names:	1-nitrophenanthrene
Inchi:	InChI=1S/C14H9NO2/c16-15(17)14-7-3-6-12-11-5-2-1-4-10(11)8-9-13(12)14/h1-9H
InchiKey:	SGNWFFATVZVHNF-UHFFFAOYSA-N
Formula:	C14H9NO2
SMILES:	O=[N+]([O-])c1cccc2c1ccc1ccccc12
Mol. weight [g/mol]:	223.23
CAS:	17024-17-8

Physical Properties

Property code	Value	Unit	Source
gf	409.00	kJ/mol	Joback Method
hf	252.68	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	3.901		Crippen Method
mcvol	162.860	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	353.40		NIST Webbook
rinpol	366.10		NIST Webbook
tb	746.16	K	Joback Method
tc	1021.21	K	Joback Method
tf	508.01	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.33	J/mol×K	746.16	Joback Method
cpg	436.51	J/mol×K	792.00	Joback Method
cpg	447.68	J/mol×K	837.84	Joback Method
cpg	458.00	J/mol×K	883.68	Joback Method
cpg	467.67	J/mol×K	929.53	Joback Method
cpg	476.86	J/mol×K	975.37	Joback Method

cpg	485.75	J/mol×K	1021.21	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=C17024178&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

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