1-Methyl-9-nitrophenanthrene

Inchi: InChI=1S/C15H11NO2/c1-10-5-4-8-12-11-6-2-3-7-13(11)15(16(17)18)9-14(10)12/h2-9H,
InchiKey: FDXNCIJOOLPXJW-UHFFFAOYSA-N
Formula: C15H11NO2
SMILES: Cc1cccc2c1cc([N+](=O)[O-])c1ccccc12
Mol. weight [g/mol]: 237.25
CAS: 87517-97-3

Physical Properties

Property code	Value	Unit	Source
gf	407.79	kJ/mol	Joback Method
hf	220.57	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	73.12	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.210		Crippen Method
mcvol	176.950	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	384.47		NIST Webbook
rinpol	383.95		NIST Webbook
rinpol	384.47		NIST Webbook
tb	774.02	K	Joback Method
tc	1042.99	K	Joback Method
tf	531.80	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.29	J/mol×K	774.02	Joback Method
cpg	486.98	J/mol×K	818.85	Joback Method
cpg	498.71	J/mol×K	863.68	Joback Method
cpg	509.65	J/mol×K	908.51	Joback Method
cpg	519.97	J/mol×K	953.34	Joback Method
cpg	529.81	J/mol×K	998.17	Joback Method

cpg	539.36	J/mol×K	1042.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87517973&Units=SI

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