1-Nitroanthraquinone

Other names:	1-Nitroanthrachinon
	1-nitro-9,10-anthracenedione
	9,10-Anthracenedione, 1-nitro-
	Anthraquinone, 1-nitro-
	«alpha»-Nitroanthraquinone
Inchi:	InChI=1S/C14H7NO4/c16-13-8-4-1-2-5-9(8)14(17)12-10(13)6-3-7-11(12)15(18)19/h1-7H
InchiKey:	YCANAXVBJKNANM-UHFFFAOYSA-N
Formula:	C14H7NO4
SMILES:	O=C1c2ccccc2C(=O)c2c1cccc2[N+](=O)[O-]
Mol. weight [g/mol]:	253.21
CAS:	82-34-8

Physical Properties

Property code	Value	Unit	Source
gf	133.86	kJ/mol	Joback Method
hf	-80.50	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	78.43	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	2.370		Crippen Method
mcvol	170.300	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	394.38		NIST Webbook
rinpol	394.38		NIST Webbook
tb	882.64	K	Joback Method
tc	1172.56	K	Joback Method
tf	643.69	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.16	J/mol×K	882.64	Joback Method
cpg	498.00	J/mol×K	930.96	Joback Method

cpg	507.52	J/mol×K	979.28	Joback Method
cpg	515.80	J/mol×K	1027.60	Joback Method
cpg	522.88	J/mol×K	1075.92	Joback Method
cpg	528.82	J/mol×K	1124.24	Joback Method
cpg	533.67	J/mol×K	1172.56	Joback Method
hsubt	139.70	kJ/mol	423.50	NIST Webbook
hsubt	108.90 ± 2.10	kJ/mol	396.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 1-aminoanthraquinone and 1-nitroanthraquinone in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.jct.2016.09.032
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=C82348&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
hsubt:	Enthalpy of sublimation 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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