1(2H)-Naphthalenone, 3,4-dihydro-7-nitro-

Other names:	7-Nitro-1-tetralone
	3,4-Dihydro-7-nitro-1(2H)-naphthalenone
	3,4-dihydro-7-nitronaphthalen-1(2H)-one
Inchi:	InChI=1S/C10H9NO3/c12-10-3-1-2-7-4-5-8(11(13)14)6-9(7)10/h4-6H,1-3H2
InchiKey:	GWAQYWSNCVEJMW-UHFFFAOYSA-N
Formula:	C10H9NO3
SMILES:	O=C1CCCc2ccc([N+](=O)[O-])cc21
Mol. weight [g/mol]:	191.18
CAS:	40353-34-2

Physical Properties

Property code	Value	Unit	Source
gf	95.79	kJ/mol	Joback Method
hf	-97.62	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	62.69	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.114		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	314.27		NIST Webbook
rinpol	314.27		NIST Webbook
rinpol	314.16		NIST Webbook
tb	700.18	K	Joback Method
tc	973.96	K	Joback Method
tf	484.41	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.00	J/mol×K	700.18	Joback Method
cpg	375.56	J/mol×K	745.81	Joback Method
cpg	387.94	J/mol×K	791.44	Joback Method

cpg	399.19	J/mol×K	837.07	Joback Method
cpg	409.35	J/mol×K	882.70	Joback Method
cpg	418.48	J/mol×K	928.33	Joback Method
cpg	426.62	J/mol×K	973.96	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=C40353342&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