Naphthalene, 1,2,3,4-tetrahydro-5-nitro-

Other names: 5-Nitro-1,2,3,4-tetrahydronaphthalene
1,2,3,4-tetrahydro-5-nitronaphthalene
Inchi: InChI=1S/C10H11NO2/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h3,5,7H,1-2,4,6H2
InchiKey: VXZHOWCMXKLZNY-UHFFFAOYSA-N
Formula: C10H11NO2
SMILES: O=[N+]([O-])c1cccc2c1CCCC2
Mol. weight [g/mol]: 177.20
CAS: 29809-14-1

Physical Properties

Property code	Value	Unit	Source
gf	218.38	kJ/mol	Joback Method
hf	40.08	kJ/mol	Joback Method
hfus	21.24	kJ/mol	Joback Method
hvap	58.44	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.474		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
rinpol	270.64		NIST Webbook
rinpol	268.52		NIST Webbook
rinpol	262.41		NIST Webbook
rinpol	270.98		NIST Webbook
rinpol	270.61		NIST Webbook
rinpol	270.98		NIST Webbook
tb	632.36	K	Joback Method
tc	894.37	K	Joback Method
tf	416.19	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.54	J/mol×K	632.36	Joback Method

cpg	355.07	J/mol×K	676.03	Joback Method
cpg	368.38	J/mol×K	719.70	Joback Method
cpg	380.59	J/mol×K	763.36	Joback Method
cpg	391.78	J/mol×K	807.03	Joback Method
cpg	402.06	J/mol×K	850.70	Joback Method
cpg	411.54	J/mol×K	894.37	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=C29809141&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