o-Nitrobenzylidene-5,6,7,8-tetrahydronaphthyl-2-a

Inchi: InChI=1S/C19H16N2O2/c20-13-18(12-17-7-3-4-8-19(17)21(22)23)16-10-9-14-5-1-2-6-15
InchiKey: KNJQLLOVNUGNDQ-LDADJPATSA-N
Formula: C19H16N2O2
SMILES: N#CC(=Cc1ccccc1[N+](=O)[O-])c1ccc2c(c1)CCCC2
Mol. weight [g/mol]: 304.34
CAS: 21848-10-2

Physical Properties

Property code	Value	Unit	Source
chs	-9853.70	kJ/mol	NIST Webbook
gf	601.79	kJ/mol	Joback Method
hf	351.69	kJ/mol	Joback Method
hfs	90.33	kJ/mol	NIST Webbook
hfus	38.60	kJ/mol	Joback Method
hvap	91.93	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	4.538		Crippen Method
mcvol	234.690	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
tb	976.06	K	Joback Method
tc	1253.76	K	Joback Method
tf	602.51	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.26	J/mol×K	976.06	Joback Method
cpg	726.30	J/mol×K	1022.34	Joback Method
cpg	738.67	J/mol×K	1068.63	Joback Method
cpg	750.59	J/mol×K	1114.91	Joback Method
cpg	762.26	J/mol×K	1161.19	Joback Method
cpg	773.88	J/mol×K	1207.47	Joback Method
cpg	785.68	J/mol×K	1253.76	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=C21848102&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume