5-Nitroacenaphthenone-1

Inchi: InChI=1S/C12H7NO3/c14-11-6-7-4-5-10(13(15)16)8-2-1-3-9(11)12(7)8/h1-5H,6H2
InchiKey: KSISVVBHVWCKOY-UHFFFAOYSA-N
Formula: C12H7NO3
SMILES: O=C1Cc2ccc([N+](=O)[O-])c3cccc1c23
Mol. weight [g/mol]: 213.19
CAS: 5386-11-8

Physical Properties

Property code	Value	Unit	Source
gf	233.85	kJ/mol	Joback Method
hf	53.02	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	2.487		Crippen Method
mcvol	144.850	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	761.36	K	Joback Method
tc	1037.39	K	Joback Method
tf	559.21	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.79	J/mol×K	761.36	Joback Method
cpg	397.89	J/mol×K	807.36	Joback Method
cpg	408.13	J/mol×K	853.37	Joback Method
cpg	417.66	J/mol×K	899.37	Joback Method
cpg	426.60	J/mol×K	945.38	Joback Method
cpg	435.10	J/mol×K	991.38	Joback Method
cpg	443.28	J/mol×K	1037.39	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=C5386118&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume