[(Z)-2-nitroethenyl]benzene

Inchi: InChI=1S/C8H7NO2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-7H/b7-6-
InchiKey: PIAOLBVUVDXHHL-SREVYHEPSA-N
Formula: C8H7NO2
SMILES: O=[N+]([O-])C=Cc1ccccc1
Mol. weight [g/mol]: 149.15

Physical Properties

Property code	Value	Unit	Source
gf	244.66	kJ/mol	Joback Method
hf	134.54	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	52.23	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.934		Crippen Method
mcvol	112.940	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	565.12	K	Joback Method
tc	820.37	K	Joback Method
tf	344.87	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.26	J/mol×K	565.12	Joback Method
cpg	258.06	J/mol×K	607.66	Joback Method
cpg	268.84	J/mol×K	650.20	Joback Method
cpg	278.67	J/mol×K	692.75	Joback Method
cpg	287.64	J/mol×K	735.29	Joback Method
cpg	295.84	J/mol×K	777.83	Joback Method
cpg	303.34	J/mol×K	820.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6002351&Units=SI
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

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