1-Nitro-2-phenylethane

Other names: (2-nitroethyl)benzene
Benzene, (2-nitroethyl)-
Inchi: InChI=1S/C8H9NO2/c10-9(11)7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey: XAWCLWKTUKMCMO-UHFFFAOYSA-N
Formula: C8H9NO2
SMILES: O=[N+]([O-])CCc1ccccc1
Mol. weight [g/mol]: 151.16
CAS: 6125-24-2

Physical Properties

Property code	Value	Unit	Source
gf	164.44	kJ/mol	Joback Method
hf	17.32	kJ/mol	Joback Method
hfus	21.88	kJ/mol	Joback Method
hvap	52.27	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.506		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
rinpol	1262.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1305.70		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1304.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2032.00		NIST Webbook
tb	560.96	K	Joback Method
tc	804.48	K	Joback Method
tf	349.95	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.02	J/mol×K	560.96	Joback Method
cpg	278.59	J/mol×K	601.55	Joback Method
cpg	290.21	J/mol×K	642.13	Joback Method
cpg	300.94	J/mol×K	682.72	Joback Method
cpg	310.82	J/mol×K	723.30	Joback Method
cpg	319.91	J/mol×K	763.89	Joback Method
cpg	328.26	J/mol×K	804.48	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55677e+01
Coeff. B	-4.70527e+03
Coeff. C	-8.65860e+01
Temperature range (K), min.	394.52
Temperature range (K), max.	545.36

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=C6125242&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume