Benzeneethanol, 4-nitro-

Other names:	Phenethyl alcohol, p-nitro-
	p-Nitrophenethyl alcohol
	2-(p-Nitrophenyl)ethanol
	4-Nitrophenethyl alcohol
	2-(4-Nitrophenyl)ethanol
Inchi:	InChI=1S/C8H9NO3/c10-6-5-7-1-3-8(4-2-7)9(11)12/h1-4,10H,5-6H2
InchiKey:	IKMXRUOZUUKSON-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	O=[N+]([O-])c1ccc(CCO)cc1
Mol. weight [g/mol]:	167.16
CAS:	100-27-6

Physical Properties

Property code	Value	Unit	Source
gf	17.99	kJ/mol	Joback Method
hf	-146.38	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	69.61	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.130		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	658.12	K	Joback Method
tc	881.82	K	Joback Method
tf	423.29	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.91	J/mol×K	658.12	Joback Method
cpg	318.61	J/mol×K	695.40	Joback Method
cpg	327.62	J/mol×K	732.69	Joback Method
cpg	335.99	J/mol×K	769.97	Joback Method

cpg	343.74	J/mol×K	807.26	Joback Method
cpg	350.92	J/mol×K	844.54	Joback Method
cpg	357.55	J/mol×K	881.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.20	K	2.10	NIST Webbook

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=C100276&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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