Benzeneethanol, 2-nitro-

Other names:	2-Nitrobenzeneethanol
	2-Nitrophenethyl alcohol
	Phenethyl alcohol, o-nitro-
	2-(o-Nitrophenyl)ethanol
	2-(o-Nitrophenyl)ethyl alcohol
Inchi:	InChI=1S/C8H9NO3/c10-6-5-7-3-1-2-4-8(7)9(11)12/h1-4,10H,5-6H2
InchiKey:	SLRIOXRBAPBGEI-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	O=[N+]([O-])c1ccccc1CCO
Mol. weight [g/mol]:	167.16
CAS:	15121-84-3

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	540.20	K	NIST Webbook
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

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=C15121843&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

Latest version available from:
https://www.chemeo.com/cid/40-510-0/Benzeneethanol-2-nitro.pdf
Generated by Cheméo on 2024-10-12 06:30:29.335463722 +0000 UTC m=+3295491.972432969.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.