2-(4-Nitrophenoxy)ethanol

Other names:	2-(p-Nitrophenoxy)ethanol
	Ethanol, 2-(4-nitrophenoxy)-
	«beta»-Hydroxyethyl p-nitrophenyl ether
	p-Nitrophenoxyethanol
	Ethanol, 2-(p-nitrophenoxy)-
Inchi:	InChI=1S/C8H9NO4/c10-5-6-13-8-3-1-7(2-4-8)9(11)12/h1-4,10H,5-6H2
InchiKey:	YAPAEYFBLRVUMH-UHFFFAOYSA-N
Formula:	C8H9NO4
SMILES:	O=[N+]([O-])c1ccc(OCCO)cc1
Mol. weight [g/mol]:	183.16
CAS:	16365-27-8

Physical Properties

Property code	Value	Unit	Source
gf	-87.01	kJ/mol	Joback Method
hf	-278.60	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	0.966		Crippen Method
mcvol	128.980	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	680.54	K	Joback Method
tc	901.43	K	Joback Method
tf	445.52	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.45	J/mol×K	680.54	Joback Method
cpg	341.05	J/mol×K	717.36	Joback Method
cpg	349.99	J/mol×K	754.17	Joback Method
cpg	358.27	J/mol×K	790.99	Joback Method

cpg	365.93	J/mol×K	827.80	Joback Method
cpg	372.97	J/mol×K	864.62	Joback Method
cpg	379.42	J/mol×K	901.43	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=C16365278&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