Benzamide, 4-nitro-N-ethyl-N-methyl-

Inchi: InChI=1S/C10H12N2O3/c1-3-11(2)10(13)8-4-6-9(7-5-8)12(14)15/h4-7H,3H2,1-2H3
InchiKey: QFUPVKZFMKXFJP-UHFFFAOYSA-N
Formula: C10H12N2O3
SMILES: CCN(C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 208.21

Physical Properties

Property code	Value	Unit	Source
gf	153.51	kJ/mol	Joback Method
hf	-80.48	kJ/mol	Joback Method
hfus	31.29	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.687		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	678.01	K	Joback Method
tc	915.04	K	Joback Method
tf	467.41	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.55	J/mol×K	678.01	Joback Method
cpg	421.31	J/mol×K	717.52	Joback Method
cpg	433.07	J/mol×K	757.02	Joback Method
cpg	443.90	J/mol×K	796.53	Joback Method
cpg	453.84	J/mol×K	836.03	Joback Method
cpg	462.96	J/mol×K	875.54	Joback Method
cpg	471.31	J/mol×K	915.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415284&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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