Benzamide, 4-nitro-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C13H18N2O3/c1-4-14(9-10(2)3)13(16)11-5-7-12(8-6-11)15(17)18/h5-8,10H,4,9
InchiKey: PTYTUOSZTQYFEG-UHFFFAOYSA-N
Formula: C13H18N2O3
SMILES: CCN(CC(C)C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	176.33	kJ/mol	Joback Method
hf	-147.68	kJ/mol	Joback Method
hfus	35.54	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.713		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	746.21	K	Joback Method
tc	974.51	K	Joback Method
tf	486.22	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.60	J/mol×K	746.21	Joback Method
cpg	579.02	J/mol×K	784.26	Joback Method
cpg	592.36	J/mol×K	822.31	Joback Method
cpg	604.68	J/mol×K	860.36	Joback Method
cpg	616.06	J/mol×K	898.41	Joback Method
cpg	626.55	J/mol×K	936.46	Joback Method
cpg	636.21	J/mol×K	974.51	Joback Method

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=U415287&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume