Benzamide, 4-nitro-N-ethyl-N-butyl-

Inchi: InChI=1S/C13H18N2O3/c1-3-5-10-14(4-2)13(16)11-6-8-12(9-7-11)15(17)18/h6-9H,3-5,1
InchiKey: CGBLXOJNDWCYPE-UHFFFAOYSA-N
Formula: C13H18N2O3
SMILES: CCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	178.77	kJ/mol	Joback Method
hf	-142.40	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.857		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2185.00		NIST Webbook
rinpol	2185.00		NIST Webbook
tb	746.65	K	Joback Method
tc	970.97	K	Joback Method
tf	501.22	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.03	J/mol×K	746.65	Joback Method
cpg	578.18	J/mol×K	784.04	Joback Method
cpg	591.31	J/mol×K	821.42	Joback Method
cpg	603.47	J/mol×K	858.81	Joback Method
cpg	614.73	J/mol×K	896.19	Joback Method
cpg	625.14	J/mol×K	933.58	Joback Method
cpg	634.76	J/mol×K	970.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415288&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