Benzamide, 4-nitro-N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C14H20N2O3/c1-4-15(10-9-11(2)3)14(17)12-5-7-13(8-6-12)16(18)19/h5-8,11H
InchiKey: YCZHIXQBXJZEKK-UHFFFAOYSA-N
Formula: C14H20N2O3
SMILES: CCN(CCC(C)C)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	184.75	kJ/mol	Joback Method
hf	-168.32	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.103		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
tb	769.09	K	Joback Method
tc	993.76	K	Joback Method
tf	497.49	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.79	J/mol×K	769.09	Joback Method
cpg	633.52	J/mol×K	806.54	Joback Method
cpg	647.17	J/mol×K	843.98	Joback Method
cpg	659.81	J/mol×K	881.43	Joback Method
cpg	671.49	J/mol×K	918.87	Joback Method
cpg	682.29	J/mol×K	956.32	Joback Method
cpg	692.27	J/mol×K	993.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415289&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