Benzamide, 4-nitro-N-ethyl-N-2-ethylhexyl-

Inchi: InChI=1S/C17H26N2O3/c1-4-7-8-14(5-2)13-18(6-3)17(20)15-9-11-16(12-10-15)19(21)22
InchiKey: OTKFHTVWHBPCBI-UHFFFAOYSA-N
Formula: C17H26N2O3
SMILES: CCCCC(CC)CN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	210.01	kJ/mol	Joback Method
hf	-230.24	kJ/mol	Joback Method
hfus	45.90	kJ/mol	Joback Method
hvap	81.37	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.273		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2489.00		NIST Webbook
rinpol	2489.00		NIST Webbook
tb	837.73	K	Joback Method
tc	1054.83	K	Joback Method
tf	531.30	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.45	J/mol×K	837.73	Joback Method
cpg	802.87	J/mol×K	873.91	Joback Method
cpg	817.22	J/mol×K	910.10	Joback Method
cpg	830.55	J/mol×K	946.28	Joback Method
cpg	842.94	J/mol×K	982.46	Joback Method
cpg	854.45	J/mol×K	1018.65	Joback Method
cpg	865.15	J/mol×K	1054.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415292&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

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