Benzamide, 4-nitro-N-ethyl-N-decyl-

Inchi: InChI=1S/C19H30N2O3/c1-3-5-6-7-8-9-10-11-16-20(4-2)19(22)17-12-14-18(15-13-17)21
InchiKey: KWQMMTIEEAXDGM-UHFFFAOYSA-N
Formula: C19H30N2O3
SMILES: CCCCCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	229.29	kJ/mol	Joback Method
hf	-266.24	kJ/mol	Joback Method
hfus	54.60	kJ/mol	Joback Method
hvap	86.21	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.198		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	883.93	K	Joback Method
tc	1097.07	K	Joback Method
tf	568.84	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.80	J/mol×K	883.93	Joback Method
cpg	919.50	J/mol×K	919.45	Joback Method
cpg	934.13	J/mol×K	954.98	Joback Method
cpg	947.78	J/mol×K	990.50	Joback Method
cpg	960.51	J/mol×K	1026.02	Joback Method
cpg	972.40	J/mol×K	1061.55	Joback Method
cpg	983.51	J/mol×K	1097.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415296&Units=SI

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