Benzamide, 4-nitro-N-ethyl-N-nonyl-

Inchi: InChI=1S/C18H28N2O3/c1-3-5-6-7-8-9-10-15-19(4-2)18(21)16-11-13-17(14-12-16)20(22
InchiKey: MTXMXQYNYDCBIB-UHFFFAOYSA-N
Formula: C18H28N2O3
SMILES: CCCCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
gf	220.87	kJ/mol	Joback Method
hf	-245.60	kJ/mol	Joback Method
hfus	52.01	kJ/mol	Joback Method
hvap	83.98	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.808		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2806.00		NIST Webbook
rinpol	2806.00		NIST Webbook
tb	861.05	K	Joback Method
tc	1074.46	K	Joback Method
tf	557.57	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.95	J/mol×K	861.05	Joback Method
cpg	860.42	J/mol×K	896.62	Joback Method
cpg	874.84	J/mol×K	932.19	Joback Method
cpg	888.28	J/mol×K	967.75	Joback Method
cpg	900.81	J/mol×K	1003.32	Joback Method
cpg	912.50	J/mol×K	1038.89	Joback Method
cpg	923.40	J/mol×K	1074.46	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=U415295&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