Benzamide, 4-nitro-N-ethyl-N-dodecyl-

Inchi: InChI=1S/C21H34N2O3/c1-3-5-6-7-8-9-10-11-12-13-18-22(4-2)21(24)19-14-16-20(17-15
InchiKey: ALQDBMBOCXVQOK-UHFFFAOYSA-N
Formula: C21H34N2O3
SMILES: CCCCCCCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 362.51

Physical Properties

Property code	Value	Unit	Source
gf	246.13	kJ/mol	Joback Method
hf	-307.52	kJ/mol	Joback Method
hfus	59.78	kJ/mol	Joback Method
hvap	90.66	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.978		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	3337.00		NIST Webbook
rinpol	3337.00		NIST Webbook
tb	929.69	K	Joback Method
tc	1144.59	K	Joback Method
tf	591.38	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.73	J/mol×K	929.69	Joback Method
cpg	1039.90	J/mol×K	965.51	Joback Method
cpg	1054.99	J/mol×K	1001.32	Joback Method
cpg	1069.08	J/mol×K	1037.14	Joback Method
cpg	1082.24	J/mol×K	1072.95	Joback Method
cpg	1094.55	J/mol×K	1108.77	Joback Method
cpg	1106.10	J/mol×K	1144.59	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=U415298&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