Benzamide, 4-nitro-N-ethyl-N-octyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	212.45	kJ/mol	Joback Method
hf	-224.96	kJ/mol	Joback Method
hfus	49.42	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.417		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	838.17	K	Joback Method
tc	1052.54	K	Joback Method
tf	546.30	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.90	J/mol×K	838.17	Joback Method
cpg	802.15	J/mol×K	873.90	Joback Method
cpg	816.36	J/mol×K	909.63	Joback Method
cpg	829.59	J/mol×K	945.36	Joback Method
cpg	841.91	J/mol×K	981.09	Joback Method
cpg	853.39	J/mol×K	1016.81	Joback Method
cpg	864.08	J/mol×K	1052.54	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=U415294&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