Benzamide, 4-nitro-N-ethyl-N-propyl-

Inchi: InChI=1S/C12H16N2O3/c1-3-9-13(4-2)12(15)10-5-7-11(8-6-10)14(16)17/h5-8H,3-4,9H2,
InchiKey: MEZZOOOCCIIBLN-UHFFFAOYSA-N
Formula: C12H16N2O3
SMILES: CCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 236.27

Physical Properties

Property code	Value	Unit	Source
gf	170.35	kJ/mol	Joback Method
hf	-121.76	kJ/mol	Joback Method
hfus	36.47	kJ/mol	Joback Method
hvap	70.62	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.467		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	723.77	K	Joback Method
tc	951.89	K	Joback Method
tf	489.95	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.96	J/mol×K	723.77	Joback Method
cpg	524.73	J/mol×K	761.79	Joback Method
cpg	537.48	J/mol×K	799.81	Joback Method
cpg	549.27	J/mol×K	837.83	Joback Method
cpg	560.15	J/mol×K	875.85	Joback Method
cpg	570.19	J/mol×K	913.87	Joback Method
cpg	579.45	J/mol×K	951.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415286&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