

Benzamide, 4-nitro-N-ethyl-N-pentyl-

Inchi:	InChI=1S/C14H20N2O3/c1-3-5-6-11-15(4-2)14(17)12-7-9-13(10-8-12)16(18)19/h7-10H,3
InchiKey:	KRAJOTDZIBMEKU-UHFFFAOYSA-N
Formula:	C14H20N2O3
SMILES:	CCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	264.32

Physical Properties

Property code	Value	Unit	Source
gf	187.19	kJ/mol	Joback Method
hf	-163.04	kJ/mol	Joback Method
hfus	41.65	kJ/mol	Joback Method
hvap	75.08	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.247		Crippen Method
mvol	213.330	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	769.53	K	Joback Method
tc	990.53	K	Joback Method
tf	512.49	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.22	J/molxK	769.53	Joback Method
cpg	632.71	J/molxK	806.36	Joback Method
cpg	646.16	J/molxK	843.20	Joback Method
cpg	658.64	J/molxK	880.03	Joback Method
cpg	670.22	J/molxK	916.86	Joback Method
cpg	680.94	J/molxK	953.70	Joback Method
cpg	690.88	J/molxK	990.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U415290&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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