Benzamide, 4-nitro-N-ethyl-N-undecyl-

Inchi: InChI=1S/C20H32N2O3/c1-3-5-6-7-8-9-10-11-12-17-21(4-2)20(23)18-13-15-19(16-14-18
InchiKey: NJRUHVPKYFXPDH-UHFFFAOYSA-N
Formula: C20H32N2O3
SMILES: CCCCCCCCCCCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	237.71	kJ/mol	Joback Method
hf	-286.88	kJ/mol	Joback Method
hfus	57.19	kJ/mol	Joback Method
hvap	88.43	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.588		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	906.81	K	Joback Method
tc	1120.43	K	Joback Method
tf	580.11	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.41	J/mol×K	906.81	Joback Method
cpg	979.34	J/mol×K	942.41	Joback Method
cpg	994.19	J/mol×K	978.02	Joback Method
cpg	1008.05	J/mol×K	1013.62	Joback Method
cpg	1020.99	J/mol×K	1049.22	Joback Method
cpg	1033.09	J/mol×K	1084.83	Joback Method
cpg	1044.41	J/mol×K	1120.43	Joback Method

Sources

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=U415297&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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