Benzamide, 4-nitro-N,N-diethyl-

Inchi: InChI=1S/C11H14N2O3/c1-3-12(4-2)11(14)9-5-7-10(8-6-9)13(15)16/h5-8H,3-4H2,1-2H3
InchiKey: JLZWKZDHHREXTA-UHFFFAOYSA-N
Formula: C11H14N2O3
SMILES: CCN(CC)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 222.24

Physical Properties

Property code	Value	Unit	Source
gf	161.93	kJ/mol	Joback Method
hf	-101.12	kJ/mol	Joback Method
hfus	33.88	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.077		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	2071.00		NIST Webbook
rinpol	2071.00		NIST Webbook
tb	700.89	K	Joback Method
tc	933.26	K	Joback Method
tf	478.68	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.11	J/mol×K	700.89	Joback Method
cpg	472.42	J/mol×K	739.62	Joback Method
cpg	484.72	J/mol×K	778.35	Joback Method
cpg	496.06	J/mol×K	817.07	Joback Method
cpg	506.51	J/mol×K	855.80	Joback Method
cpg	516.13	J/mol×K	894.53	Joback Method
cpg	524.96	J/mol×K	933.26	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=U415285&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