Benzamide, N-(2-nitrophenyl)-

Other names:	o'-Nitrobenzanilide
	Benzanilide, 2'-nitro-
	N-(o-Nitrophenyl)benzamide
	2-Nitro-N-benzoylaniline
	2'-Nitrobenzanilide
Inchi:	InChI=1S/C13H10N2O3/c16-13(10-6-2-1-3-7-10)14-11-8-4-5-9-12(11)15(17)18/h1-9H,(H
InchiKey:	ARMSTQBMUHJXHU-UHFFFAOYSA-N
Formula:	C13H10N2O3
SMILES:	O=C(Nc1ccccc1[N+](=O)[O-])c1ccccc1
Mol. weight [g/mol]:	242.23
CAS:	728-90-5

Physical Properties

Property code	Value	Unit	Source
gf	269.79	kJ/mol	Joback Method
hf	80.07	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	79.52	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	2.847		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
tb	811.06	K	Joback Method
tc	1078.56	K	Joback Method
tf	547.83	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.46	J/mol×K	811.06	Joback Method
cpg	492.83	J/mol×K	855.64	Joback Method
cpg	503.02	J/mol×K	900.23	Joback Method
cpg	512.13	J/mol×K	944.81	Joback Method

cpg	520.26	J/mol×K	989.39	Joback Method
cpg	527.51	J/mol×K	1033.98	Joback Method
cpg	533.99	J/mol×K	1078.56	Joback Method

Sources

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=C728905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume