N-(2-Nitro-phenyl)-benzamide

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

Physical Properties

Property code	Value	Unit	Source
hf	17.36	kJ/mol	Cheméo Relay (1.0)
hfus	35.18	kJ/mol	Joback Method
hvap	97.91	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-4.06		Cheméo Relay (1.0)
logp	2.847		Crippen Method
mcvol	175.480	ml/mol	McGowan Method
tb	618.84	K	Cheméo Relay (1.0)
tf	420.05	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C728905&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point