

3-Nitro-4-chlorobenzanilide

Other names:	Benzamide, 4-chloro-3-nitro-N-phenyl- 4-Chloro-3-nitro-N-phenylbenzamide
Inchi:	InChI=1S/C13H9ClN2O3/c14-11-7-6-9(8-12(11)16(18)19)13(17)15-10-4-2-1-3-5-10/h1-8
InchiKey:	MPSDMWLZVDJFGW-UHFFFAOYSA-N
Formula:	C13H9ClN2O3
SMILES:	O=C(Nc1ccccc1)c1ccc(Cl)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	276.68

Physical Properties

Property code	Value	Unit	Source
hfus	38.99	kJ/mol	Joback Method
hvap	99.99	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-4.57		Cheméo Relay (1.0)
logp	3.500		Crippen Method
mcvol	187.720	ml/mol	McGowan Method
tb	633.86	K	Cheméo Relay (1.0)
tf	411.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.61	J/mol×K	853.47	Joback Method
cpg	508.57	J/mol×K	898.35	Joback Method
cpg	517.46	J/mol×K	943.23	Joback Method
cpg	525.35	J/mol×K	988.11	Joback Method
cpg	532.35	J/mol×K	1032.99	Joback Method
cpg	538.56	J/mol×K	1077.87	Joback Method
cpg	544.05	J/mol×K	1122.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41614168&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
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

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