

N-(2-CHLORO-4-NITROPHENYL)BENZAMIDE

Other names:	N-(2-Chloro-4-nitrophenyl)benzamide 3-Chloro-4-benzamido-nitrobenzene
Inchi:	InChI=1S/C13H9ClN2O3/c14-11-8-10(16(18)19)6-7-12(11)15-13(17)9-4-2-1-3-5-9/h1-8H
InchiKey:	BCTFYSXVHA FEGT-UHFFFAOYSA-N
Formula:	C13H9ClN2O3
SMILES:	O=C(Nc1ccc([N+](=O)[O-])cc1Cl)c1ccccc1
Mol. weight [g/mol]:	276.68

Physical Properties

Property code	Value	Unit	Source
hfus	38.99	kJ/mol	Joback Method
hvap	107.37	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-4.56		Cheméo Relay (1.0)
logp	3.500		Crippen Method
mcvol	187.720	ml/mol	McGowan Method
tb	624.43	K	Cheméo Relay (1.0)
tf	429.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.66	J/mol×K	853.67	Joback Method
cpg	508.62	J/mol×K	898.56	Joback Method
cpg	517.50	J/mol×K	943.45	Joback Method
cpg	525.39	J/mol×K	988.34	Joback Method
cpg	532.39	J/mol×K	1033.23	Joback Method
cpg	538.59	J/mol×K	1078.12	Joback Method
cpg	544.09	J/mol×K	1123.01	Joback Method

Sources

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=C64160389&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

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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