4-Chloro-3-nitrobenzanilide

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
CAS:	41614-16-8

Physical Properties

Property code	Value	Unit	Source
gf	248.23	kJ/mol	Joback Method
hf	52.86	kJ/mol	Joback Method
hfus	38.99	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.500		Crippen Method
mcvol	187.720	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	853.47	K	Joback Method
tc	1122.75	K	Joback Method
tf	590.27	K	Joback Method
vc	0.720	m3/kmol	Joback Method

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

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=C41614168&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

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