Benzamide, 2-chloro-n-cyanomethyl-4-nitro-n-phenyl-

Inchi: InChI=1S/C15H10ClN3O3/c16-14-10-12(19(21)22)6-7-13(14)15(20)18(9-8-17)11-4-2-1-3

InchiKey: GOAPRVVYNWEGBW-UHFFFAOYSA-N

Formula: C15H10ClN3O3

SMILES: N#CCN(C(=O)c1ccc([N+](=O)[O-])cc1Cl)c1ccccc1

Mol. weight [g/mol]: 315.71

CAS: 22977-96-4

Physical Properties

Property code	Value	Unit	Source
gf	419.64	kJ/mol	Joback Method
hf	190.52	kJ/mol	Joback Method
hfus	43.59	kJ/mol	Joback Method
hvap	95.10	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.419		Crippen Method
mcvol	217.280	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	963.58	K	Joback Method
tc	1229.61	K	Joback Method
tf	657.61	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.14	J/mol×K	963.58	Joback Method
cpg	609.52	J/mol×K	1007.92	Joback Method
cpg	617.05	J/mol×K	1052.26	Joback Method
cpg	623.83	J/mol×K	1096.60	Joback Method
cpg	629.97	J/mol×K	1140.93	Joback Method
cpg	635.60	J/mol×K	1185.27	Joback Method
cpg	640.83	J/mol×K	1229.61	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=C22977964&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