Benzamide, 2-chloro-n-(cyanomethyl)-n-ethyl-4-nitro-

Inchi: InChI=1S/C11H10ClN3O3/c1-2-14(6-5-13)11(16)9-4-3-8(15(17)18)7-10(9)12/h3-4,7H,2,6

InchiKey: WENFSKFNPFSJPQ-UHFFFAOYSA-N

Formula: C11H10ClN3O3

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

Mol. weight [g/mol]: 267.67

CAS: 22977-88-4

Physical Properties

Property code	Value	Unit	Source
gf	273.55	kJ/mol	Joback Method
hf	36.55	kJ/mol	Joback Method
hfus	39.19	kJ/mol	Joback Method
hvap	83.92	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.234		Crippen Method
mcvol	184.680	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
tb	845.38	K	Joback Method
tc	1090.78	K	Joback Method
tf	586.11	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.36	J/mol×K	845.38	Joback Method
cpg	499.36	J/mol×K	886.28	Joback Method
cpg	507.53	J/mol×K	927.18	Joback Method
cpg	514.95	J/mol×K	968.08	Joback Method
cpg	521.67	J/mol×K	1008.98	Joback Method
cpg	527.75	J/mol×K	1049.88	Joback Method
cpg	533.26	J/mol×K	1090.78	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=C22977884&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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