N-(2-cyanoethyl)-4-nitrobenzamide

Inchi: InChI=1S/C10H9N3O3/c11-6-1-7-12-10(14)8-2-4-9(5-3-8)13(15)16/h2-5H,1,7H2,(H,12,14
InchiKey: IWRJJZIUBZXAMG-UHFFFAOYSA-N
Formula: C10H9N3O3
SMILES: N#CCCNC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 219.20
CAS: 1141-61-3

Physical Properties

Property code	Value	Unit	Source
gf	265.30	kJ/mol	Joback Method
hf	70.34	kJ/mol	Joback Method
hfus	34.87	kJ/mol	Joback Method
hvap	81.04	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	1.238		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	817.82	K	Joback Method
tc	1065.84	K	Joback Method
tf	552.59	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.86	J/mol×K	817.82	Joback Method
cpg	437.79	J/mol×K	859.16	Joback Method
cpg	445.89	J/mol×K	900.49	Joback Method
cpg	453.21	J/mol×K	941.83	Joback Method
cpg	459.80	J/mol×K	983.17	Joback Method
cpg	465.72	J/mol×K	1024.50	Joback Method
cpg	471.01	J/mol×K	1065.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1141613&Units=SI

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