Benzamide,n-[2-(2-cyano)propyl]-2-chloro-4-nitro-

Inchi: InChI=1S/C11H10ClN3O3/c1-11(2,6-13)14-10(16)8-4-3-7(15(17)18)5-9(8)12/h3-5H,1-2H
InchiKey: UBQKIFJOOGUFPP-UHFFFAOYSA-N
Formula: C11H10ClN3O3
SMILES: CC(C)(C#N)NC(=O)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]: 267.67
CAS: 22977-97-5

Physical Properties

Property code	Value	Unit	Source
gf	255.00	kJ/mol	Joback Method
hf	13.74	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	2.280		Crippen Method
mcvol	184.680	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	879.88	K	Joback Method
tc	1137.96	K	Joback Method
tf	608.72	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.94	J/mol×K	879.88	Joback Method
cpg	507.37	J/mol×K	922.89	Joback Method
cpg	515.02	J/mol×K	965.91	Joback Method
cpg	521.97	J/mol×K	1008.92	Joback Method
cpg	528.32	J/mol×K	1051.93	Joback Method
cpg	534.16	J/mol×K	1094.95	Joback Method
cpg	539.59	J/mol×K	1137.96	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=C22977975&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