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

Inchi: InChI=1S/C12H12ClN3O3/c1-2-6-15(7-5-14)12(17)10-4-3-9(16(18)19)8-11(10)13/h3-4,8

InchiKey: YPTXIFWZSOODGM-UHFFFAOYSA-N

Formula: C12H12ClN3O3

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

Mol. weight [g/mol]: 281.69

CAS: 22977-93-1

Physical Properties

Property code	Value	Unit	Source
gf	281.97	kJ/mol	Joback Method
hf	15.91	kJ/mol	Joback Method
hfus	41.78	kJ/mol	Joback Method
hvap	86.15	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.624		Crippen Method
mcvol	198.770	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
tb	868.26	K	Joback Method
tc	1109.74	K	Joback Method
tf	597.38	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.85	J/mol×K	868.26	Joback Method
cpg	553.32	J/mol×K	908.51	Joback Method
cpg	561.95	J/mol×K	948.75	Joback Method
cpg	569.82	J/mol×K	989.00	Joback Method
cpg	576.98	J/mol×K	1029.25	Joback Method
cpg	583.49	J/mol×K	1069.50	Joback Method
cpg	589.41	J/mol×K	1109.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22977931&Units=SI
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

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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