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

Inchi: InChI=1S/C13H14ClN3O3/c1-2-3-7-16(8-6-15)13(18)11-5-4-10(17(19)20)9-12(11)14/h4-5

InchiKey: RTNZVWIHJYVKOO-UHFFFAOYSA-N

Formula: C13H14ClN3O3

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

Mol. weight [g/mol]: 295.72

CAS: 22977-94-2

Physical Properties

Property code	Value	Unit	Source
gf	290.39	kJ/mol	Joback Method
hf	-4.73	kJ/mol	Joback Method
hfus	44.37	kJ/mol	Joback Method
hvap	88.37	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.014		Crippen Method
mcvol	212.860	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
tb	891.14	K	Joback Method
tc	1129.38	K	Joback Method
tf	608.65	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.31	J/mol×K	891.14	Joback Method
cpg	608.19	J/mol×K	930.85	Joback Method
cpg	617.24	J/mol×K	970.55	Joback Method
cpg	625.50	J/mol×K	1010.26	Joback Method
cpg	633.05	J/mol×K	1049.97	Joback Method
cpg	639.94	J/mol×K	1089.68	Joback Method
cpg	646.25	J/mol×K	1129.38	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=C22977942&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