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

Inchi: InChI=1S/C13H14ClN3O4/c1-2-21-8-7-16(6-5-15)13(18)11-4-3-10(17(19)20)9-12(11)14/
InchiKey: BCJZEQOLPOOXSP-UHFFFAOYSA-N
Formula: C13H14ClN3O4
SMILES: CCOCCN(CC#N)C(=O)c1ccc([N+](=O)[O-])cc1Cl
Mol. weight [g/mol]: 311.72
CAS: 22978-00-3

Physical Properties

Property code	Value	Unit	Source
gf	185.39	kJ/mol	Joback Method
hf	-136.95	kJ/mol	Joback Method
hfus	45.56	kJ/mol	Joback Method
hvap	90.79	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.250		Crippen Method
mcvol	218.730	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
tb	913.56	K	Joback Method
tc	1150.05	K	Joback Method
tf	630.88	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.62	J/mol×K	913.56	Joback Method
cpg	631.98	J/mol×K	952.97	Joback Method
cpg	640.41	J/mol×K	992.39	Joback Method
cpg	647.94	J/mol×K	1031.80	Joback Method
cpg	654.62	J/mol×K	1071.22	Joback Method
cpg	660.49	J/mol×K	1110.63	Joback Method
cpg	665.59	J/mol×K	1150.05	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=C22978003&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