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

Inchi: InChI=1S/C12H10ClN3O3/c13-11-7-9(16(18)19)3-4-10(11)12(17)15(6-5-14)8-1-2-8/h3-4,
InchiKey: SCHJGZHAVVNDDB-UHFFFAOYSA-N
Formula: C12H10ClN3O3
SMILES: N#CCN(C(=O)c1ccc([N+](=O)[O-])cc1Cl)C1CC1
Mol. weight [g/mol]: 279.68
CAS: 22977-92-0

Physical Properties

Property code	Value	Unit	Source
gf	342.72	kJ/mol	Joback Method
hf	88.71	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	86.06	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	2.376		Crippen Method
mcvol	187.910	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
tb	875.00	K	Joback Method
tc	1129.47	K	Joback Method
tf	615.32	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.21	J/mol×K	875.00	Joback Method
cpg	534.82	J/mol×K	917.41	Joback Method
cpg	543.71	J/mol×K	959.82	Joback Method
cpg	552.01	J/mol×K	1002.24	Joback Method
cpg	559.82	J/mol×K	1044.65	Joback Method
cpg	567.26	J/mol×K	1087.06	Joback Method
cpg	574.47	J/mol×K	1129.47	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=C22977920&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