4-Chloro-n,n-bis(2-cyanoethyl)benzamide

Inchi: InChI=1S/C13H12ClN3O/c14-12-5-3-11(4-6-12)13(18)17(9-1-7-15)10-2-8-16/h3-6H,1-2,9
InchiKey: ZLBDPVOLPCUMQY-UHFFFAOYSA-N
Formula: C13H12ClN3O
SMILES: N#CCCN(CCC#N)C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 261.71
CAS: 106472-11-1

Physical Properties

Property code	Value	Unit	Source
gf	397.65	kJ/mol	Joback Method
hf	182.38	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.610		Crippen Method
mcvol	196.820	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
tb	836.40	K	Joback Method
tc	1066.73	K	Joback Method
tf	517.51	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.44	J/mol×K	836.40	Joback Method
cpg	530.88	J/mol×K	874.79	Joback Method
cpg	539.57	J/mol×K	913.18	Joback Method
cpg	547.55	J/mol×K	951.56	Joback Method
cpg	554.90	J/mol×K	989.95	Joback Method
cpg	561.66	J/mol×K	1028.34	Joback Method
cpg	567.89	J/mol×K	1066.73	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=C106472111&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