2-Chloro-n-(2-cyanoethyl)benzamide

Inchi: InChI=1S/C10H9ClN2O/c11-9-5-2-1-4-8(9)10(14)13-7-3-6-12/h1-2,4-5H,3,7H2,(H,13,14)
InchiKey: JEQATADDGNMFCW-UHFFFAOYSA-N
Formula: C10H9ClN2O
SMILES: N#CCCNC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 208.64
CAS: 22192-81-0

Physical Properties

Property code	Value	Unit	Source
gf	217.82	kJ/mol	Joback Method
hf	65.36	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	68.84	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	1.983		Crippen Method
mcvol	153.170	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	703.41	K	Joback Method
tc	936.10	K	Joback Method
tf	438.90	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.59	J/mol×K	703.41	Joback Method
cpg	376.42	J/mol×K	742.19	Joback Method
cpg	385.50	J/mol×K	780.97	Joback Method
cpg	393.85	J/mol×K	819.76	Joback Method
cpg	401.52	J/mol×K	858.54	Joback Method
cpg	408.54	J/mol×K	897.32	Joback Method
cpg	414.96	J/mol×K	936.10	Joback Method

Sources

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=C22192810&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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