

N,n-bis(2-cyanoethyl)-4-nitrobenzamide

Inchi:	InChI=1S/C13H12N4O3/c14-7-1-9-16(10-2-8-15)13(18)11-3-5-12(6-4-11)17(19)20/h3-6H
InchiKey:	BYJIYCDZRXINKP-UHFFFAOYSA-N
Formula:	C13H12N4O3
SMILES:	N#CCCN(CCC#N)C(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	272.26
CAS:	100725-06-2

Physical Properties

Property code	Value	Unit	Source
gf	445.13	kJ/mol	Joback Method
hf	187.36	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	93.81	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	1.864		Crippen Method
mcvol	202.000	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
tb	950.81	K	Joback Method
tc	1196.00	K	Joback Method
tf	631.20	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.86	J/molxK	950.81	Joback Method
cpg	593.10	J/molxK	991.68	Joback Method
cpg	600.59	J/molxK	1032.54	Joback Method
cpg	607.41	J/molxK	1073.41	Joback Method
cpg	613.64	J/molxK	1114.27	Joback Method
cpg	619.33	J/molxK	1155.14	Joback Method
cpg	624.58	J/molxK	1196.00	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=C100725062&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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