

Formamide, N,N-bis(2-cyanoethyl)-

Other names:	N,N-Bis(2-cyanoethyl)formamide N,N-Bis(«beta»-cyanoethyl)-formamide 3,3'-Formyliminodipropionitrile
Inchi:	InChI=1S/C7H9N3O/c8-3-1-5-10(7-11)6-2-4-9/h7H,1-2,5-6H2
InchiKey:	MYRFNYCEQURXPT-UHFFFAOYSA-N
Formula:	C7H9N3O
SMILES:	N#CCCN(C=O)CCC#N
Mol. weight [g/mol]:	151.17
CAS:	3445-84-9

Physical Properties

Property code	Value	Unit	Source
gf	285.68	kJ/mol	Joback Method
hf	123.90	kJ/mol	Joback Method
hfus	22.21	kJ/mol	Joback Method
hvap	60.89	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.272		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
tb	624.82	K	Joback Method
tc	829.94	K	Joback Method
tf	373.10	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.85	J/molxK	624.82	Joback Method
cpg	304.04	J/molxK	659.01	Joback Method
cpg	311.74	J/molxK	693.19	Joback Method
cpg	318.96	J/molxK	727.38	Joback Method
cpg	325.73	J/molxK	761.57	Joback Method
cpg	332.07	J/molxK	795.75	Joback Method

Sources

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=C3445849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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