

Acetonitrile, 2,2'-iminobis-

Other names:	Acetonitrile, iminodi- Iminodiacetonitrile 1,1'-Imidodiacetonitrile Di(cianometil)ammina 2406 I.S.
Inchi:	InChI=1S/C4H5N3/c5-1-3-7-4-2-6/h7H,3-4H2
InchiKey:	BSRDNMMLQYNQQD-UHFFFAOYSA-N
Formula:	C4H5N3
SMILES:	N#CCNCC#N
Mol. weight [g/mol]:	95.10
CAS:	628-87-5

Physical Properties

Property code	Value	Unit	Source
gf	338.55	kJ/mol	Joback Method
hf	257.34	kJ/mol	Joback Method
hfus	14.23	kJ/mol	Joback Method
hvap	51.89	kJ/mol	Joback Method
log10ws	-0.42		Crippen Method
logp	-0.377		Crippen Method
mcvol	79.960	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	545.25	K	Joback Method
tc	760.51	K	Joback Method
tf	317.48	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.68	J/molxK	545.25	Joback Method
cpg	169.39	J/molxK	581.13	Joback Method
cpg	174.79	J/molxK	617.00	Joback Method
cpg	179.88	J/molxK	652.88	Joback Method

cpg	184.68	J/mol×K	688.76	Joback Method
cpg	189.21	J/mol×K	724.64	Joback Method
cpg	193.45	J/mol×K	760.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C628875&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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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