Acetonitrile, nitrilotri-

Other names: nitrilotriacetonitrile
Inchi: InChI=1S/C6H6N4/c7-1-4-10(5-2-8)6-3-9/h4-6H2
InchiKey: LJAIDEYQVIJERM-UHFFFAOYSA-N
Formula: C6H6N4
SMILES: N#CCN(CC#N)CC#N
Mol. weight [g/mol]: 134.14
CAS: 7327-60-8

Physical Properties

Property code	Value	Unit	Source
gf	509.96	kJ/mol	Joback Method
hf	395.00	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	62.43	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	-0.141		Crippen Method
mcvol	109.520	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	655.36	K	Joback Method
tc	874.80	K	Joback Method
tf	384.82	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.57	J/mol×K	655.36	Joback Method
cpg	256.97	J/mol×K	691.93	Joback Method
cpg	262.96	J/mol×K	728.51	Joback Method
cpg	268.54	J/mol×K	765.08	Joback Method
cpg	273.74	J/mol×K	801.65	Joback Method
cpg	278.58	J/mol×K	838.23	Joback Method
cpg	283.10	J/mol×K	874.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7327608&Units=SI
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

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