

Acetonitrile, (methylenedinitrilo)tetra-

Inchi:	InChI=1S/C9H10N6/c10-1-5-14(6-2-11)9-15(7-3-12)8-4-13/h5-9H2
InchiKey:	WJGXTAWLNPYQFI-UHFFFAOYSA-N
Formula:	C9H10N6
SMILES:	N#CCN(CC#N)CN(CC#N)CC#N
Mol. weight [g/mol]:	202.22
CAS:	1116-43-4

Physical Properties

Property code	Value	Unit	Source
gf	779.18	kJ/mol	Joback Method
hf	565.49	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	81.63	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	-0.358		Crippen Method
mcvol	163.150	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
tb	838.52	K	Joback Method
tc	1058.03	K	Joback Method
tf	516.09	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.66	J/molxK	838.52	Joback Method
cpg	444.78	J/molxK	875.10	Joback Method
cpg	451.41	J/molxK	911.69	Joback Method
cpg	457.58	J/molxK	948.27	Joback Method
cpg	463.35	J/molxK	984.86	Joback Method
cpg	468.75	J/molxK	1021.44	Joback Method
cpg	473.82	J/molxK	1058.03	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=C1116434&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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