

1,1,2,2-Cyclopropane-tetracarbonitrile

Other names:	1,1,2,2-Tetracyanocyclopropane
Inchi:	InChI=1S/C7H2N4/c8-2-6(3-9)1-7(6,4-10)5-11/h1H2
InchiKey:	PSDKLXIWEMMSLZ-UHFFFAOYSA-N
Formula:	C7H2N4
SMILES:	N#CC1(C#N)CC1(C#N)C#N
Mol. weight [g/mol]:	142.12
CAS:	2424-32-0

Physical Properties

Property code	Value	Unit	Source
chs	-3639.00 ± 10.00	kJ/mol	NIST Webbook
gf	582.84	kJ/mol	Joback Method
hf	554.65	kJ/mol	Joback Method
hfs	596.00 ± 10.00	kJ/mol	NIST Webbook
hfus	6.52	kJ/mol	Joback Method
hvap	70.39	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	0.457		Crippen Method
mcvol	104.150	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
tb	770.43	K	Joback Method
tc	1032.46	K	Joback Method
tf	490.11	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.32	J/molxK	770.43	Joback Method
cpg	244.56	J/molxK	814.10	Joback Method
cpg	251.87	J/molxK	857.77	Joback Method
cpg	260.61	J/molxK	901.44	Joback Method
cpg	271.13	J/molxK	945.12	Joback Method
cpg	283.80	J/molxK	988.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2424320&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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