

2,4,6-Cycloheptatriene-1-carbonitrile

Other names:	1,3,5-Cycloheptatriene-7-carbonitrile 2,4,6-Cycloheptatrienecarbonitrile 7-Cyano-1,3,5-cycloheptatriene 7-Cyanocycloheptatriene 1-Cyano-2,4,6-cycloheptatriene 7-cyanotropilidene
Inchi:	InChI=1S/C8H7N/c9-7-8-5-3-1-2-4-6-8/h1-6,8H
InchiKey:	LADCKIXFXIKHQM-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	N#CC1C=CC=CC=C1
Mol. weight [g/mol]:	117.15
CAS:	13612-59-4

Physical Properties

Property code	Value	Unit	Source
gf	251.89	kJ/mol	Joback Method
hf	177.93	kJ/mol	Joback Method
hfus	11.38	kJ/mol	Joback Method
hvap	45.36	kJ/mol	Joback Method
ie	8.89	eV	NIST Webbook
log10ws	-2.25		Crippen Method
logp	1.808		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	505.82	K	Joback Method
tc	745.17	K	Joback Method
tf	251.05	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.17	J/molxK	505.82	Joback Method
cpg	215.33	J/molxK	545.71	Joback Method

cpg	226.66	J/mol×K	585.60	Joback Method
cpg	237.18	J/mol×K	625.50	Joback Method
cpg	246.92	J/mol×K	665.39	Joback Method
cpg	255.91	J/mol×K	705.28	Joback Method
cpg	264.16	J/mol×K	745.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13612594&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

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
h vap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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