

Cyclohexane, 1,2,4-tris(methylene)-

Inchi:	InChI=1S/C9H12/c1-7-4-5-8(2)9(3)6-7/h1-6H2
InchiKey:	AMBNQWVPTPHADI-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C=C1CCC(=C)C(=C)C1
Mol. weight [g/mol]:	120.19
CAS:	14296-81-2

Physical Properties

Property code	Value	Unit	Source
gf	216.30	kJ/mol	Joback Method
hf	98.29	kJ/mol	Joback Method
hfus	6.35	kJ/mol	Joback Method
hvap	36.84	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.839		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
ripol	1297.00		NIST Webbook
tb	427.02	K	Joback Method
tc	632.01	K	Joback Method
tf	243.85	K	Joback Method
vc	0.425	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.04	J/molxK	427.02	Joback Method
cpg	275.31	J/molxK	597.84	Joback Method
cpg	264.23	J/molxK	563.68	Joback Method
cpg	252.57	J/molxK	529.51	Joback Method
cpg	240.33	J/molxK	495.35	Joback Method
cpg	227.49	J/molxK	461.18	Joback Method
cpg	285.83	J/molxK	632.01	Joback Method
dvisc	0.0002813	Paxs	427.02	Joback Method

dvisc	0.0003413	Paxs	396.49	Joback Method
dvisc	0.0004277	Paxs	365.96	Joback Method
dvisc	0.0005585	Paxs	335.44	Joback Method
dvisc	0.0007692	Paxs	304.91	Joback Method
dvisc	0.0011377	Paxs	274.38	Joback Method
dvisc	0.0018559	Paxs	243.85	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=C14296812&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
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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