

cis,trans,cis-1,2,3,4-Tetravinylcyclobutane

Inchi:	InChI=1S/C12H16/c1-5-9-10(6-2)12(8-4)11(9)7-3/h5-12H,1-4H2/t9-,10-,11-,12-
InchiKey:	XXHDKZTASMVSX-NQYKUJLISA-N
Formula:	C12H16
SMILES:	C=CC1C(C=C)C(C=C)C1C=C
Mol. weight [g/mol]:	160.26
CAS:	82865-42-7

Physical Properties

Property code	Value	Unit	Source
gf	427.04	kJ/mol	Joback Method
hf	216.33	kJ/mol	Joback Method
hfus	20.96	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
ie	9.16	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	3.209		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
tb	457.68	K	Joback Method
tc	650.76	K	Joback Method
tf	219.66	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.93	J/molxK	457.68	Joback Method
cpg	404.13	J/molxK	618.58	Joback Method
cpg	389.62	J/molxK	586.40	Joback Method
cpg	374.29	J/molxK	554.22	Joback Method
cpg	358.09	J/molxK	522.04	Joback Method
cpg	340.98	J/molxK	489.86	Joback Method
cpg	417.84	J/molxK	650.76	Joback Method

dvisc	0.0003519	Paxs	457.68	Joback Method
dvisc	0.0003619	Paxs	418.01	Joback Method
dvisc	0.0003743	Paxs	378.34	Joback Method
dvisc	0.0003901	Paxs	338.67	Joback Method
dvisc	0.0004112	Paxs	299.00	Joback Method
dvisc	0.0004404	Paxs	259.33	Joback Method
dvisc	0.0004836	Paxs	219.66	Joback Method

Sources

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=C82865427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
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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