

Cyclohexane, 1r,2c,4t-tris-ethenyl

Inchi:	InChI=1S/C12H18/c1-4-10-7-8-11(5-2)12(6-3)9-10/h4-6,10-12H,1-3,7-9H2/t10-,11-,12+/n
InchiKey:	KTRQRAQRHBLCSQ-UTUOFQBUSA-N
Formula:	C12H18
SMILES:	C=CC1CCC(C=C)C(C=C)C1
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	322.71	kJ/mol	Joback Method
hf	98.92	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	40.11	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.577		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	1114.00		NIST Webbook
tb	474.21	K	Joback Method
tc	678.46	K	Joback Method
tf	218.62	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.41	J/molxK	474.21	Joback Method
cpg	431.53	J/molxK	644.42	Joback Method
cpg	415.30	J/molxK	610.38	Joback Method
cpg	398.11	J/molxK	576.33	Joback Method
cpg	379.92	J/molxK	542.29	Joback Method
cpg	360.70	J/molxK	508.25	Joback Method
cpg	446.82	J/molxK	678.46	Joback Method
dvisc	0.0002602	Paxs	474.21	Joback Method
dvisc	0.0003121	Paxs	431.61	Joback Method

dvisc	0.0003895	Paxs	389.01	Joback Method
dvisc	0.0005134	Paxs	346.41	Joback Method
dvisc	0.0007313	Paxs	303.82	Joback Method
dvisc	0.0011689	Paxs	261.22	Joback Method
dvisc	0.0022430	Paxs	218.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R10913&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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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