

Cyclohexene, 4-ethenyl-1,2,4-trimethyl

Inchi:	InChI=1S/C11H18/c1-5-11(4)7-6-9(2)10(3)8-11/h5H,1,6-8H2,2-4H3
InchiKey:	IVYYYULHFGBRLJ-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	C=CC1(C)CCC(C)=C(C)C1
Mol. weight [g/mol]:	150.26

Physical Properties

Property code	Value	Unit	Source
gf	159.24	kJ/mol	Joback Method
hf	-40.54	kJ/mol	Joback Method
hfus	8.95	kJ/mol	Joback Method
hvap	40.30	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.699		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpola	1038.00		NIST Webbook
rinpola	1038.00		NIST Webbook
tb	476.67	K	Joback Method
tc	688.77	K	Joback Method
tf	269.05	K	Joback Method
vc	0.549	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.43	J/mol×K	476.67	Joback Method
cpg	334.40	J/mol×K	512.02	Joback Method
cpg	351.24	J/mol×K	547.37	Joback Method
cpg	367.06	J/mol×K	582.72	Joback Method
cpg	381.96	J/mol×K	618.07	Joback Method
cpg	396.06	J/mol×K	653.42	Joback Method
cpg	409.45	J/mol×K	688.77	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=R128015&Units=SI

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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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