

Cyclohexene, 2-ethenyl-1,3,3-trimethyl-

Inchi:	InChI=1S/C11H18/c1-5-10-9(2)7-6-8-11(10,3)4/h5H,1,6-8H2,2-4H3
InchiKey:	LWYKRZJSOCUPJG-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]:	150.26
CAS:	5293-90-3

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
tb	476.67	K	Joback Method
tc	688.77	K	Joback Method
tf	269.05	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.43	J/molxK	476.67	Joback Method
cpg	334.40	J/molxK	512.02	Joback Method
cpg	351.24	J/molxK	547.37	Joback Method
cpg	367.06	J/molxK	582.72	Joback Method
cpg	381.96	J/molxK	618.07	Joback Method
cpg	396.06	J/molxK	653.42	Joback Method
cpg	409.45	J/molxK	688.77	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=C5293903&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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