

Cyclohexene, 1,2,4-trimethyl-4-(1-methylethenyl)-

Inchi:	InChI=1S/C12H20/c1-9(2)12(5)7-6-10(3)11(4)8-12/h1,6-8H2,2-5H3
InchiKey:	HNXIHAQWIOOZSF-UHFFFAOYSA-N
Formula:	C12H20
SMILES:	C=C(C)C1(C)CCC(C)=C(C)C1
Mol. weight [g/mol]:	164.29
CAS:	16195-58-7

Physical Properties

Property code	Value	Unit	Source
gf	159.11	kJ/mol	Joback Method
hf	-70.97	kJ/mol	Joback Method
hfus	10.23	kJ/mol	Joback Method
hvap	42.61	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	4.089		Crippen Method
mcvol	160.480	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	499.43	K	Joback Method
tc	712.45	K	Joback Method
tf	266.36	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.51	J/mol×K	499.43	Joback Method
cpg	381.49	J/mol×K	534.93	Joback Method
cpg	399.31	J/mol×K	570.44	Joback Method
cpg	416.09	J/mol×K	605.94	Joback Method
cpg	431.94	J/mol×K	641.44	Joback Method
cpg	446.96	J/mol×K	676.95	Joback Method
cpg	461.27	J/mol×K	712.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16195587&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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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