

Cyclohexene, 1,4-dimethyl-4-(1-methylethenyl)

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

Physical Properties

Property code	Value	Unit	Source
gf	160.32	kJ/mol	Joback Method
hf	-38.86	kJ/mol	Joback Method
hfus	8.03	kJ/mol	Joback Method
hvap	39.72	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.699		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
tb	471.57	K	Joback Method
tc	686.57	K	Joback Method
tf	242.57	K	Joback Method
vc	0.550	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.14	J/mol×K	471.57	Joback Method
cpg	333.91	J/mol×K	507.40	Joback Method
cpg	351.42	J/mol×K	543.24	Joback Method
cpg	367.81	J/mol×K	579.07	Joback Method
cpg	383.19	J/mol×K	614.91	Joback Method
cpg	397.67	J/mol×K	650.74	Joback Method
cpg	411.38	J/mol×K	686.57	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=R127998&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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