

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

Inchi:	InChI=1S/C11H18/c1-8(2)11-6-5-9(3)10(4)7-11/h11H,1,5-7H2,2-4H3
InchiKey:	DJNBXADZJNAMQR-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	C=C(C)C1CCC(C)=C(C)C1
Mol. weight [g/mol]:	150.26

Physical Properties

Property code	Value	Unit	Source
gf	156.18	kJ/mol	Joback Method
hf	-65.57	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	41.54	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.699		Crippen Method
mcvol	146.390	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
rinpol	1119.00		NIST Webbook
rinpol	1119.00		NIST Webbook
tb	476.31	K	Joback Method
tc	683.55	K	Joback Method
tf	231.19	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.76	J/mol×K	476.31	Joback Method
cpg	333.86	J/mol×K	510.85	Joback Method
cpg	351.06	J/mol×K	545.39	Joback Method
cpg	367.39	J/mol×K	579.93	Joback Method
cpg	382.87	J/mol×K	614.47	Joback Method
cpg	397.53	J/mol×K	649.01	Joback Method
cpg	411.39	J/mol×K	683.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R127983&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
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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