

4-methyl-3-carene

Inchi:	InChI=1S/C11H18/c1-7-5-9-10(6-8(7)2)11(9,3)4/h9-10H,5-6H2,1-4H3
InchiKey:	VRGXZSITWYAVQT-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	CC1=C(C)CC2C(C1)C2(C)C
Mol. weight [g/mol]:	150.26

Physical Properties

Property code	Value	Unit	Source
gf	148.64	kJ/mol	Joback Method
hf	-101.19	kJ/mol	Joback Method
hfus	13.63	kJ/mol	Joback Method
hvap	40.23	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.389		Crippen Method
mcvol	139.830	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinqol	1074.00		NIST Webbook
tb	473.52	K	Joback Method
tc	681.25	K	Joback Method
tf	291.55	K	Joback Method
vc	0.540	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.61	J/mol×K	473.52	Joback Method
cpg	338.85	J/mol×K	508.14	Joback Method
cpg	355.85	J/mol×K	542.76	Joback Method
cpg	371.74	J/mol×K	577.39	Joback Method
cpg	386.64	J/mol×K	612.01	Joback Method
cpg	400.69	J/mol×K	646.63	Joback Method
cpg	414.01	J/mol×K	681.25	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=R492178&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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