

cis-4-carene

Inchi:	InChI=1S/C10H16/c1-7-4-5-8-9(6-7)10(8,2)3/h4-5,7-9H,6H2,1-3H3/t7-,8+,9-/m0/s1
InchiKey:	LGNSZMLHOYDATP-YIZRAAEISA-N
Formula:	C10H16
SMILES:	CC1C=CC2C(C1)C2(C)C
Mol. weight [g/mol]:	136.23

Physical Properties

Property code	Value	Unit	Source
gf	151.77	kJ/mol	Joback Method
hf	-77.95	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	36.38	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.855		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
tb	436.01	K	Joback Method
tc	643.39	K	Joback Method
tf	251.00	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.63	J/mol×K	436.01	Joback Method
cpg	291.69	J/mol×K	470.57	Joback Method
cpg	309.35	J/mol×K	505.14	Joback Method
cpg	325.74	J/mol×K	539.70	Joback Method
cpg	340.98	J/mol×K	574.26	Joback Method
cpg	355.22	J/mol×K	608.83	Joback Method
cpg	368.57	J/mol×K	643.39	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492207&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
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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