

cis-4-methylcarene

Inchi:	InChI=1S/C11H18/c1-7-5-9-10(6-8(7)2)11(9,3)4/h5,8-10H,6H2,1-4H3/t8-,9-,10+/m0/s1
InchiKey:	BNCOXEAHDQARFK-LPEHRKFASA-N
Formula:	C11H18
SMILES:	CC1=CC2C(CC1C)C2(C)C
Mol. weight [g/mol]:	150.26

Physical Properties

Property code	Value	Unit	Source
gf	150.56	kJ/mol	Joback Method
hf	-110.06	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	39.26	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.245		Crippen Method
mcvol	139.830	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	1004.00		NIST Webbook
rinpol	1004.00		NIST Webbook
tb	463.87	K	Joback Method
tc	670.00	K	Joback Method
tf	274.79	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.40	J/mol×K	463.87	Joback Method
cpg	338.54	J/mol×K	498.23	Joback Method
cpg	356.39	J/mol×K	532.58	Joback Method
cpg	373.06	J/mol×K	566.94	Joback Method
cpg	388.69	J/mol×K	601.29	Joback Method
cpg	403.39	J/mol×K	635.65	Joback Method
cpg	417.29	J/mol×K	670.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R492212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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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