1,1,2,4-tetramethylcyclopentane, trans,cis

Inchi: InChI=1S/C9H18/c1-7-5-8(2)9(3,4)6-7/h7-8H,5-6H2,1-4H3/t7-,8-/m1/s1
InchiKey: AVBGIJNNMIBMQG-HTQZYQBOSA-N
Formula: C9H18
SMILES: CC1CC(C)C(C)(C)C1
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	40.54	kJ/mol	Joback Method
hf	-194.05	kJ/mol	Joback Method
hfus	8.84	kJ/mol	Joback Method
hvap	34.12	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	816.50		NIST Webbook
rinpol	816.50		NIST Webbook
tb	411.50	K	Joback Method
tc	610.26	K	Joback Method
tf	217.51	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.44	J/mol×K	411.50	Joback Method
cpg	275.25	J/mol×K	444.63	Joback Method
cpg	292.94	J/mol×K	477.75	Joback Method
cpg	309.58	J/mol×K	510.88	Joback Method
cpg	325.27	J/mol×K	544.01	Joback Method
cpg	340.08	J/mol×K	577.14	Joback Method
cpg	354.09	J/mol×K	610.26	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=R141107&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume