trans-1,1,2,3-Tetramethylcyclopentane

Other names: 1,1,2-trans-3-tetramethylcyclopentane
Inchi: InChI=1S/C9H18/c1-7-5-6-9(3,4)8(7)2/h7-8H,5-6H2,1-4H3/t7-,8+/m0/s1
InchiKey: CXCBKSYSKZEEJB-JGVFFNPUSA-N
Formula: C9H18
SMILES: CC1CCC(C)(C)C1C
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	811.00		NIST Webbook
rinpol	820.00		NIST Webbook
rinpol	818.00		NIST Webbook
rinpol	815.00		NIST Webbook
rinpol	814.00		NIST Webbook
rinpol	811.00		NIST Webbook
rinpol	820.80		NIST Webbook
rinpol	815.30		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:	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=R92951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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