3,3,5,5-Tetramethylcyclopentene

Inchi: InChI=1S/C9H16/c1-8(2)5-6-9(3,4)7-8/h5-6H,7H2,1-4H3
InchiKey: FCJMCOVEXBZEMH-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1(C)C=CC(C)(C)C1
Mol. weight [g/mol]: 124.22
CAS: 38667-10-6

Physical Properties

Property code	Value	Unit	Source
gf	72.72	kJ/mol	Joback Method
hf	-100.69	kJ/mol	Joback Method
hfus	2.70	kJ/mol	Joback Method
hvap	33.57	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	852.00		NIST Webbook
tb	380.18 ± 0.50	K	NIST Webbook
tc	626.15	K	Joback Method
tf	208.92 ± 0.30	K	NIST Webbook
tf	208.92 ± 0.50	K	NIST Webbook
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.07	J/mol×K	415.57	Joback Method
cpg	262.06	J/mol×K	450.67	Joback Method
cpg	278.49	J/mol×K	485.76	Joback Method
cpg	293.55	J/mol×K	520.86	Joback Method
cpg	307.40	J/mol×K	555.96	Joback Method
cpg	320.25	J/mol×K	591.05	Joback Method
cpg	332.27	J/mol×K	626.15	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=C38667106&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
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