2,6-Dimethyl-2,5-heptadiene

Inchi: InChI=1S/C9H16/c1-8(2)6-5-7-9(3)4/h6-7H,5H2,1-4H3
InchiKey: WCMUAGGUXKQBSS-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC(C)=CCC=C(C)C
Mol. weight [g/mol]: 124.22

Physical Properties

Property code	Value	Unit	Source
gf	168.24	kJ/mol	Joback Method
hf	-14.23	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	35.70	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.309		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	905.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	413.40	K	Joback Method
tc	600.31	K	Joback Method
tf	153.11	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.17	J/mol×K	413.40	Joback Method
cpg	257.46	J/mol×K	444.55	Joback Method
cpg	271.01	J/mol×K	475.70	Joback Method
cpg	283.86	J/mol×K	506.86	Joback Method
cpg	296.05	J/mol×K	538.01	Joback Method

cpg	307.60	J/mol×K	569.16	Joback Method
cpg	318.56	J/mol×K	600.31	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=C6090160&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