2,4-Heptadiene, 2,6-dimethyl-

Other names: 2,6-dimethyl-2,4-heptadiene
Inchi: InChI=1S/C9H16/c1-8(2)6-5-7-9(3)4/h5-8H,1-4H3/b6-5+
InchiKey: HQTKNGJJNNTBLG-AATRIKPKSA-N
Formula: C9H16
SMILES: CC(C)=CC=CC(C)C
Mol. weight [g/mol]: 124.22
CAS: 4634-87-1

Physical Properties

Property code	Value	Unit	Source
gf	174.35	kJ/mol	Joback Method
hf	-9.72	kJ/mol	Joback Method
hfus	14.64	kJ/mol	Joback Method
hvap	35.24	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
tb	413.08	K	Joback Method
tc	600.66	K	Joback Method
tf	152.07	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.19	J/mol×K	413.08	Joback Method
cpg	257.66	J/mol×K	444.34	Joback Method
cpg	271.38	J/mol×K	475.61	Joback Method
cpg	284.38	J/mol×K	506.87	Joback Method
cpg	296.71	J/mol×K	538.13	Joback Method
cpg	308.40	J/mol×K	569.40	Joback Method
cpg	319.47	J/mol×K	600.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4634871&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume