1,6-Heptadiene, 3,3-dimethyl-

Inchi: InChI=1S/C9H16/c1-5-7-8-9(3,4)6-2/h5-6H,1-2,7-8H2,3-4H3
InchiKey: YWOCVROBRVNVFV-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=CCCC(C)(C)C=C
Mol. weight [g/mol]: 124.22
CAS: 68701-61-1

Physical Properties

Property code	Value	Unit	Source
gf	203.42	kJ/mol	Joback Method
hf	13.02	kJ/mol	Joback Method
hfus	9.09	kJ/mol	Joback Method
hvap	32.99	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.165		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
tb	395.45	K	Joback Method
tc	576.29	K	Joback Method
tf	190.09	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.47	J/mol×K	395.45	Joback Method
cpg	309.33	J/mol×K	546.15	Joback Method
cpg	297.57	J/mol×K	516.01	Joback Method
cpg	285.13	J/mol×K	485.87	Joback Method
cpg	271.99	J/mol×K	455.73	Joback Method
cpg	258.12	J/mol×K	425.59	Joback Method
cpg	320.45	J/mol×K	576.29	Joback Method
dvisc	0.0002576	Pa×s	395.45	Joback Method
dvisc	0.0003490	Pa×s	361.22	Joback Method

dvisc	0.0005040	Pa×s	327.00	Joback Method
dvisc	0.0007931	Pa×s	292.77	Joback Method
dvisc	0.0014073	Pa×s	258.54	Joback Method
dvisc	0.0029744	Pa×s	224.32	Joback Method
dvisc	0.0082311	Pa×s	190.09	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=C68701611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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