1,4-Pentadiene, 3,3-dimethyl-

Inchi: InChI=1S/C7H12/c1-5-7(3,4)6-2/h5-6H,1-2H2,3-4H3
InchiKey: BHZUNHXTRRNKST-UHFFFAOYSA-N
Formula: C7H12
SMILES: C=CC(C)(C)C=C
Mol. weight [g/mol]: 96.17
CAS: 1112-35-2

Physical Properties

Property code	Value	Unit	Source
gf	186.58	kJ/mol	Joback Method
hf	54.30	kJ/mol	Joback Method
hfus	3.91	kJ/mol	Joback Method
hvap	28.54	kJ/mol	Joback Method
ie	9.55	eV	NIST Webbook
log10ws	-2.22		Crippen Method
logp	2.385		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	349.69	K	Joback Method
tc	531.89	K	Joback Method
tf	167.55	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.34	J/mol×K	349.69	Joback Method
cpg	179.69	J/mol×K	380.06	Joback Method
cpg	191.36	J/mol×K	410.42	Joback Method
cpg	202.38	J/mol×K	440.79	Joback Method
cpg	212.77	J/mol×K	471.16	Joback Method
cpg	222.57	J/mol×K	501.52	Joback Method
cpg	231.80	J/mol×K	531.89	Joback Method
dvisc	0.0075642	Pa×s	167.55	Joback Method

dvisc	0.0028149	Pa×s	197.91	Joback Method
dvisc	0.0013625	Pa×s	228.26	Joback Method
dvisc	0.0007820	Pa×s	258.62	Joback Method
dvisc	0.0005043	Pa×s	288.98	Joback Method
dvisc	0.0003535	Pa×s	319.33	Joback Method
dvisc	0.0002636	Pa×s	349.69	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=C1112352&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
ie:	Ionization energy
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