1,3-Pentadiene, 3-methyl-

Other names: 3-Methyl-1,3-pentadiene
CH3CH=C(CH3)CH=CH2
Inchi: InChI=1S/C6H10/c1-4-6(3)5-2/h4-5H,1H2,2-3H3
InchiKey: BOGRNZQRTNVZCZ-UHFFFAOYSA-N
Formula: C6H10
SMILES: C=CC(C)=CC
Mol. weight [g/mol]: 82.14
CAS: 4549-74-0

Physical Properties

Property code	Value	Unit	Source
affp	852.30	kJ/mol	NIST Webbook
basg	823.40	kJ/mol	NIST Webbook
gf	159.15	kJ/mol	Joback Method
hf	65.69	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	28.32	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.139		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	647.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	637.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	647.00		NIST Webbook
rinpol	639.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	642.00		NIST Webbook
ripol	756.00		NIST Webbook
ripol	787.00		NIST Webbook
tb	348.00 ± 3.00	K	NIST Webbook
tb	351.00 ± 4.00	K	NIST Webbook
tb	351.00 ± 2.00	K	NIST Webbook
tb	350.20	K	NIST Webbook
tb	350.00 ± 4.00	K	NIST Webbook

tc	517.19	K	Joback Method
tf	136.58	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.16	J/mol×K	337.40	Joback Method
cpg	142.08	J/mol×K	367.36	Joback Method
cpg	151.51	J/mol×K	397.33	Joback Method
cpg	160.47	J/mol×K	427.29	Joback Method
cpg	168.98	J/mol×K	457.26	Joback Method
cpg	177.07	J/mol×K	487.22	Joback Method
cpg	184.75	J/mol×K	517.19	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4549740&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

affp: Proton affinity
basg: Gas basicity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume