

1,4-Pentadiene, 2,3,4-trimethyl-

Other names:	(CH ₃) ₂ C=C(CH ₃)C(CH ₃)=CH ₂
Inchi:	InChI=1S/C8H14/c1-6(2)8(5)7(3)4/h8H,1,3H2,2,4-5H3
InchiKey:	AFQPKTBBNINMQ-UHFFFAOYSA-N
Formula:	C ₈ H ₁₄
SMILES:	C=C(C)C(C)C(=C)C
Mol. weight [g/mol]:	110.20
CAS:	72014-90-5

Physical Properties

Property code	Value	Unit	Source
affp	869.90	kJ/mol	NIST Webbook
basg	841.00	kJ/mol	NIST Webbook
gf	172.62	kJ/mol	Joback Method
hf	17.55	kJ/mol	Joback Method
hfus	7.77	kJ/mol	Joback Method
hvap	31.83	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.775		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	375.12	K	Joback Method
tc	556.50	K	Joback Method
tf	133.48	K	Joback Method
vc	0.442	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.24	J/mol×K	375.12	Joback Method
cpg	216.01	J/mol×K	405.35	Joback Method
cpg	228.20	J/mol×K	435.58	Joback Method
cpg	239.83	J/mol×K	465.81	Joback Method
cpg	250.92	J/mol×K	496.04	Joback Method
cpg	261.50	J/mol×K	526.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72014905&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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