

4-METHYL-1,2-PENTADIENE

Inchi:

InChI=1S/C6H10/c1-4-5-6(2)3/h5-6H,1H2,2-3H3

InchiKey:

CAAAXQFHDYHTTC-UHFFFAOYSA-N

Formula:

C6H10

SMILES:

C=C=CC(C)C

Mol. weight [g/mol]:

82.15

Physical Properties

Property code	Value	Unit	Source
gf	213.32	kJ/mol	Joback Method
hf	115.76	kJ/mol	Joback Method
hfus	8.62	kJ/mol	Joback Method
hvap	28.33	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	1.983		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	336.19	K	Joback Method
tc	518.97	K	Joback Method
tf	147.13	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.57	J/mol×K	336.19	Joback Method
cpg	148.49	J/mol×K	366.65	Joback Method
cpg	157.12	J/mol×K	397.12	Joback Method
cpg	165.46	J/mol×K	427.58	Joback Method
cpg	173.51	J/mol×K	458.04	Joback Method
cpg	181.28	J/mol×K	488.51	Joback Method
cpg	188.77	J/mol×K	518.97	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol377.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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