1-Pentyne, 3,4-dimethyl

Inchi: InChI=1S/C7H12/c1-5-7(4)6(2)3/h1,6-7H,2-4H3
InchiKey: JDQKSTIAVKXRSK-UHFFFAOYSA-N
Formula: C7H12
SMILES: C#CC(C)C(C)C
Mol. weight [g/mol]: 96.17

Physical Properties

Property code	Value	Unit	Source
gf	226.25	kJ/mol	Joback Method
hf	93.53	kJ/mol	Joback Method
hfus	9.81	kJ/mol	Joback Method
hvap	30.26	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.912		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	624.00		NIST Webbook
rinpol	624.00		NIST Webbook
tb	348.80	K	Joback Method
tc	532.81	K	Joback Method
tf	185.62	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.68	J/mol×K	348.80	Joback Method
cpg	182.74	J/mol×K	379.47	Joback Method
cpg	193.32	J/mol×K	410.14	Joback Method
cpg	203.43	J/mol×K	440.81	Joback Method
cpg	213.09	J/mol×K	471.48	Joback Method
cpg	222.30	J/mol×K	502.14	Joback Method
cpg	231.10	J/mol×K	532.81	Joback Method

Sources

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=R66540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume