1-Pentyne, 3,3-dimethyl-

Inchi: InChI=1S/C7H12/c1-5-7(3,4)6-2/h1H,6H2,2-4H3
InchiKey: KQIIKSQUHGGYCU-UHFFFAOYSA-N
Formula: C7H12
SMILES: C#CC(C)(C)CC
Mol. weight [g/mol]: 96.17
CAS: 918-82-1

Physical Properties

Property code	Value	Unit	Source
gf	233.97	kJ/mol	Joback Method
hf	95.34	kJ/mol	Joback Method
hfus	9.45	kJ/mol	Joback Method
hvap	29.74	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.056		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
rinpol	589.00		NIST Webbook
tb	346.45	K	Joback Method
tc	534.00	K	Joback Method
tf	218.04	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.38	J/mol×K	346.45	Joback Method
cpg	184.40	J/mol×K	377.71	Joback Method
cpg	195.76	J/mol×K	408.97	Joback Method
cpg	206.48	J/mol×K	440.22	Joback Method
cpg	216.60	J/mol×K	471.48	Joback Method
cpg	226.14	J/mol×K	502.74	Joback Method
cpg	235.13	J/mol×K	534.00	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol424.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C918821&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

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