2-Heptyne, 4,4-dimethyl

Inchi: InChI=1S/C9H16/c1-5-7-9(3,4)8-6-2/h5,7H2,1-4H3
InchiKey: VIQJNDDATMJYRT-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC#CC(C)(C)CCC
Mol. weight [g/mol]: 124.22
CAS: 67291-83-2

Physical Properties

Property code	Value	Unit	Source
gf	230.54	kJ/mol	Joback Method
hf	34.46	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	36.48	kJ/mol	Joback Method
ie	9.18 ± 0.01	eV	NIST Webbook
log10ws	-3.14		Crippen Method
logp	2.836		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2761.36	kPa	Joback Method
rinpol	806.00		NIST Webbook
rinpol	806.00		NIST Webbook
tb	411.09	K	Joback Method
tc	609.72	K	Joback Method
tf	299.71	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.02	J/mol×K	411.09	Joback Method
cpg	263.88	J/mol×K	444.20	Joback Method
cpg	277.98	J/mol×K	477.30	Joback Method
cpg	291.34	J/mol×K	510.41	Joback Method
cpg	303.99	J/mol×K	543.51	Joback Method
cpg	315.98	J/mol×K	576.62	Joback Method

cpg	327.33	J/mol×K	609.72	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=C67291832&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
ie:	Ionization energy
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