2-Hexyne, 4,4,5-trimethyl

Inchi: InChI=1S/C9H16/c1-6-7-9(4,5)8(2)3/h8H,1-5H3
InchiKey: YRWKVFWKGUZUGY-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC#CC(C)(C)C(C)C
Mol. weight [g/mol]: 124.22
CAS: 994-21-8

Physical Properties

Property code	Value	Unit	Source
gf	228.10	kJ/mol	Joback Method
hf	29.18	kJ/mol	Joback Method
hfus	11.25	kJ/mol	Joback Method
hvap	36.10	kJ/mol	Joback Method
ie	9.15 ± 0.01	eV	NIST Webbook
log10ws	-2.90		Crippen Method
logp	2.692		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	806.00		NIST Webbook
tb	410.65	K	Joback Method
tc	614.14	K	Joback Method
tf	284.71	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.99	J/mol×K	410.65	Joback Method
cpg	264.32	J/mol×K	444.57	Joback Method
cpg	278.83	J/mol×K	478.48	Joback Method
cpg	292.56	J/mol×K	512.40	Joback Method
cpg	305.55	J/mol×K	546.31	Joback Method
cpg	317.83	J/mol×K	580.23	Joback Method
cpg	329.43	J/mol×K	614.14	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C994218&Units=SI

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