2-Hexyne, 4,4-dimethyl

Inchi: InChI=1S/C8H14/c1-5-7-8(3,4)6-2/h6H2,1-4H3
InchiKey: DYXMSZQNXBAGJT-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC#CC(C)(C)CC
Mol. weight [g/mol]: 110.20

Physical Properties

Property code	Value	Unit	Source
gf	222.12	kJ/mol	Joback Method
hf	55.10	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	34.26	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.446		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	720.00		NIST Webbook
tb	388.21	K	Joback Method
tc	588.56	K	Joback Method
tf	288.44	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.81	J/mol×K	388.21	Joback Method
cpg	223.46	J/mol×K	421.60	Joback Method
cpg	236.39	J/mol×K	454.99	Joback Method
cpg	248.63	J/mol×K	488.38	Joback Method
cpg	260.22	J/mol×K	521.78	Joback Method
cpg	271.19	J/mol×K	555.17	Joback Method
cpg	281.56	J/mol×K	588.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66568&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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