1-Hexyne, 3,3-dimethyl

Inchi: InChI=1S/C8H14/c1-5-7-8(3,4)6-2/h2H,5,7H2,1,3-4H3
InchiKey: MLRORDXAZGLTKK-UHFFFAOYSA-N
Formula: C8H14
SMILES: C#CC(C)(C)CCC
Mol. weight [g/mol]: 110.20

Physical Properties

Property code	Value	Unit	Source
gf	242.39	kJ/mol	Joback Method
hf	74.70	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	31.96	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.446		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	679.00		NIST Webbook
rinpol	679.00		NIST Webbook
tb	369.33	K	Joback Method
tc	556.28	K	Joback Method
tf	229.31	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.60	J/mol×K	369.33	Joback Method
cpg	221.92	J/mol×K	400.49	Joback Method
cpg	234.52	J/mol×K	431.65	Joback Method
cpg	246.44	J/mol×K	462.81	Joback Method
cpg	257.70	J/mol×K	493.97	Joback Method
cpg	268.33	J/mol×K	525.12	Joback Method
cpg	278.38	J/mol×K	556.28	Joback Method

Sources

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=R66479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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