1-Hexyne, 3,5-dimethyl

Inchi: InChI=1S/C8H14/c1-5-8(4)6-7(2)3/h1,7-8H,6H2,2-4H3
InchiKey: OMKSPQSURAIMIF-UHFFFAOYSA-N
Formula: C8H14
SMILES: C#CC(C)CC(C)C
Mol. weight [g/mol]: 110.20

Physical Properties

Property code	Value	Unit	Source
gf	234.67	kJ/mol	Joback Method
hf	72.89	kJ/mol	Joback Method
hfus	12.40	kJ/mol	Joback Method
hvap	32.48	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.302		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpol	690.00		NIST Webbook
rinpol	690.00		NIST Webbook
tb	371.68	K	Joback Method
tc	555.16	K	Joback Method
tf	196.89	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.48	J/mol×K	371.68	Joback Method
cpg	219.93	J/mol×K	402.26	Joback Method
cpg	231.83	J/mol×K	432.84	Joback Method
cpg	243.21	J/mol×K	463.42	Joback Method
cpg	254.08	J/mol×K	494.00	Joback Method
cpg	264.45	J/mol×K	524.58	Joback Method
cpg	274.35	J/mol×K	555.16	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=R66497&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
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