1-Hexene, 3,5,5-trimethyl-

Other names:	3,5,5-Trimethyl-1-hexene
	3,5,5-Trimethylhexene-1
Inchi:	InChI=1S/C9H18/c1-6-8(2)7-9(3,4)5/h6,8H,1,7H2,2-5H3
InchiKey:	JTXUVHFRSRTSAT-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	C=CC(C)CC(C)(C)C
Mol. weight [g/mol]:	126.24
CAS:	4316-65-8

Physical Properties

Property code	Value	Unit	Source
gf	113.14	kJ/mol	Joback Method
hf	-117.69	kJ/mol	Joback Method
hfus	6.85	kJ/mol	Joback Method
hvap	33.27	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.245		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	770.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	766.50		NIST Webbook
rinpol	767.60		NIST Webbook
rinpol	768.70		NIST Webbook
rinpol	770.00		NIST Webbook
rinpol	771.20		NIST Webbook
rinpol	772.70		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	767.40		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	767.90		NIST Webbook
rinpol	771.90		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	765.30		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	767.00		NIST Webbook

rinpol	767.90		NIST Webbook
rinpol	768.80		NIST Webbook
rinpol	769.80		NIST Webbook
rinpol	795.00		NIST Webbook
rinpol	764.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	768.00		NIST Webbook
rinpol	768.80		NIST Webbook
rinpol	773.80		NIST Webbook
rinpol	764.00		NIST Webbook
tb	392.60 ± 5.00	K	NIST Webbook
tc	579.58	K	Joback Method
tf	176.85	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.54	J/mol×K	398.33	Joback Method
cpg	329.08	J/mol×K	549.37	Joback Method
cpg	316.41	J/mol×K	519.16	Joback Method
cpg	303.05	J/mol×K	488.95	Joback Method
cpg	288.97	J/mol×K	458.75	Joback Method
cpg	274.14	J/mol×K	428.54	Joback Method
cpg	341.10	J/mol×K	579.58	Joback Method
dvisc	0.0002526	Pa×s	398.33	Joback Method
dvisc	0.0003590	Pa×s	361.42	Joback Method
dvisc	0.0005527	Pa×s	324.50	Joback Method
dvisc	0.0009507	Pa×s	287.59	Joback Method
dvisc	0.0019184	Pa×s	250.68	Joback Method
dvisc	0.0049331	Pa×s	213.76	Joback Method
dvisc	0.0188168	Pa×s	176.85	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=C4316658&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
dvisc:	Dynamic viscosity
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