3-Hexene, 2,2,5-trimethyl

Inchi: InChI=1S/C9H18/c1-8(2)6-7-9(3,4)5/h6-8H,1-5H3/b7-6+
InchiKey: TWZONWQQRUSASE-VOTSOKGWSA-N
Formula: C9H18
SMILES: CC(C)C=CC(C)(C)C
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	105.52	kJ/mol	Joback Method
hf	-125.90	kJ/mol	Joback Method
hfus	8.33	kJ/mol	Joback Method
hvap	33.90	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.245		Crippen Method
mcvol	133.370	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	765.00		NIST Webbook
rinpol	765.00		NIST Webbook
tb	405.81	K	Joback Method
tc	592.45	K	Joback Method
tf	173.53	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.50	J/mol×K	405.81	Joback Method
cpg	275.50	J/mol×K	436.92	Joback Method
cpg	290.65	J/mol×K	468.02	Joback Method
cpg	304.97	J/mol×K	499.13	Joback Method
cpg	318.51	J/mol×K	530.24	Joback Method
cpg	331.32	J/mol×K	561.35	Joback Method
cpg	343.42	J/mol×K	592.45	Joback Method
dvisc	0.0221680	Pa×s	173.53	Joback Method

dvisc	0.0050227	Pa×s	212.24	Joback Method
dvisc	0.0017992	Pa×s	250.96	Joback Method
dvisc	0.0008480	Pa×s	289.67	Joback Method
dvisc	0.0004772	Pa×s	328.38	Joback Method
dvisc	0.0003032	Pa×s	367.10	Joback Method
dvisc	0.0002101	Pa×s	405.81	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=R127210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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