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

Inchi: InChI=1S/C9H18/c1-6-9(4,5)7-8(2)3/h6,8H,1,7H2,2-5H3
InchiKey: JWKWSKMAPDHZIR-UHFFFAOYSA-N
Formula: C9H18
SMILES: C=CC(C)(C)CC(C)C
Mol. weight [g/mol]: 126.24
CAS: 13427-43-5

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
tb	398.33	K	Joback Method
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	274.14	J/mol×K	428.54	Joback Method
cpg	288.97	J/mol×K	458.75	Joback Method
cpg	303.05	J/mol×K	488.95	Joback Method
cpg	316.41	J/mol×K	519.16	Joback Method
cpg	329.08	J/mol×K	549.37	Joback Method
cpg	341.10	J/mol×K	579.58	Joback Method
dvisc	0.0188168	Pa×s	176.85	Joback Method
dvisc	0.0049331	Pa×s	213.76	Joback Method

dvisc	0.0019184	Pa×s	250.68	Joback Method
dvisc	0.0009507	Pa×s	287.59	Joback Method
dvisc	0.0005527	Pa×s	324.50	Joback Method
dvisc	0.0003590	Pa×s	361.42	Joback Method
dvisc	0.0002526	Pa×s	398.33	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13427435&Units=SI

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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