3-Hexene, 2,2-dimethyl-

Other names: 2,2-Dimethyl-3-hexene
5,5-Dimethyl-3-hexene
2,2-dimethylhex-3-ene
Inchi: InChI=1S/C8H16/c1-5-6-7-8(2,3)4/h6-7H,5H2,1-4H3/b7-6+
InchiKey: JPLZSSHKQZJYTJ-VOTSOKGWSA-N
Formula: C8H16
SMILES: CCC=CC(C)(C)C
Mol. weight [g/mol]: 112.21
CAS: 3123-93-1

Physical Properties

Property code	Value	Unit	Source
gf	99.54	kJ/mol	Joback Method
hf	-99.98	kJ/mol	Joback Method
hfus	9.26	kJ/mol	Joback Method
hvap	32.06	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	373.25 ± 0.50	K	NIST Webbook
tb	372.65 ± 2.00	K	NIST Webbook
tc	566.77	K	Joback Method
tf	177.26	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.13	J/mol×K	383.37	Joback Method
cpg	233.64	J/mol×K	413.94	Joback Method
cpg	247.38	J/mol×K	444.50	Joback Method
cpg	260.39	J/mol×K	475.07	Joback Method
cpg	272.68	J/mol×K	505.64	Joback Method

cpg	284.31	J/mol×K	536.21	Joback Method
cpg	295.30	J/mol×K	566.77	Joback Method
dvisc	0.0110015	Pa×s	177.26	Joback Method
dvisc	0.0034054	Pa×s	211.61	Joback Method
dvisc	0.0014626	Pa×s	245.96	Joback Method
dvisc	0.0007728	Pa×s	280.31	Joback Method
dvisc	0.0004693	Pa×s	314.67	Joback Method
dvisc	0.0003144	Pa×s	349.02	Joback Method
dvisc	0.0002263	Pa×s	383.37	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=C3123931&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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