

1-Hexene, 3,3-dimethyl-

Other names:	3,3-Dimethyl-1-hexene 3,3-Dimethylhex-1-ene
Inchi:	InChI=1S/C8H16/c1-5-7-8(3,4)6-2/h6H,2,5,7H2,1,3-4H3
InchiKey:	RXYYKIMRVXDSFR-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	C=CC(C)(C)CCC
Mol. weight [g/mol]:	112.21
CAS:	3404-77-1

Physical Properties

Property code	Value	Unit	Source
gf	107.16	kJ/mol	Joback Method
hf	-91.77	kJ/mol	Joback Method
hfus	7.78	kJ/mol	Joback Method
hvap	36.00	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	713.10		NIST Webbook
rinpol	714.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	718.00		NIST Webbook
rinpol	712.30		NIST Webbook
tb	375.89	K	Joback Method
tc	553.76	K	Joback Method
tf	180.58	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.61	J/mol×K	375.89	Joback Method
cpg	232.71	J/mol×K	405.54	Joback Method

cpg	246.11	J/molxK	435.18	Joback Method
cpg	258.84	J/molxK	464.83	Joback Method
cpg	270.93	J/molxK	494.47	Joback Method
cpg	282.41	J/molxK	524.12	Joback Method
cpg	293.30	J/molxK	553.76	Joback Method
dvisc	0.0095731	Paxs	180.58	Joback Method
dvisc	0.0033567	Paxs	213.13	Joback Method
dvisc	0.0015537	Paxs	245.68	Joback Method
dvisc	0.0008612	Paxs	278.24	Joback Method
dvisc	0.0005402	Paxs	310.79	Joback Method
dvisc	0.0003702	Paxs	343.34	Joback Method
dvisc	0.0002708	Paxs	375.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.24030e+01
Coeff. B	-2.55909e+03
Coeff. C	-6.46190e+01
Temperature range (K), min.	275.85
Temperature range (K), max.	425.49

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3404771&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol286.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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