4,4-Dimethyl-1-hexene

Other names: 1-Hexene, 4,4-dimethyl-
4,4-Dimethylhex-1-ene
Inchi: InChI=1S/C8H16/c1-5-7-8(3,4)6-2/h5H,1,6-7H2,2-4H3
InchiKey: SUJVAMIXNUAJEY-UHFFFAOYSA-N
Formula: C8H16
SMILES: C=CCC(C)(C)CC
Mol. weight [g/mol]: 112.21
CAS: 1647-08-1

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	31.00	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	728.10		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	723.30		NIST Webbook
tb	375.89	K	Joback Method
tc	553.76	K	Joback Method
tf	180.58	K	Joback Method
vc	0.454	m3/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/mol×K	435.18	Joback Method
cpg	258.84	J/mol×K	464.83	Joback Method
cpg	270.93	J/mol×K	494.47	Joback Method
cpg	282.41	J/mol×K	524.12	Joback Method
cpg	293.30	J/mol×K	553.76	Joback Method
dvisc	0.0095731	Pa×s	180.58	Joback Method
dvisc	0.0033567	Pa×s	213.13	Joback Method
dvisc	0.0015537	Pa×s	245.68	Joback Method
dvisc	0.0008612	Pa×s	278.24	Joback Method
dvisc	0.0005402	Pa×s	310.79	Joback Method
dvisc	0.0003702	Pa×s	343.34	Joback Method
dvisc	0.0002708	Pa×s	375.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.26501e+01
Coeff. B	-2.64563e+03
Coeff. C	-6.39590e+01
Temperature range (K), min.	277.96
Temperature range (K), max.	424.47

Sources

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/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol289.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1647081&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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume