2-Hexene, 5,5-dimethyl-, (E)-

Other names:	(E)-5,5-Dimethyl-2-hexene
	(E)-5,5-Dimethylhex-2-ene
	5,5-Dimethyl-2-hexene (trans)
	5,5-Dimethyl-trans-2-hexene
Inchi:	InChI=1S/C8H16/c1-5-6-7-8(2,3)4/h5-6H,7H2,1-4H3/b6-5+
InchiKey:	NWZJLSKAFZXSQH-AATRIKPKSA-N
Formula:	C8H16
SMILES:	CC=CCC(C)(C)C
Mol. weight [g/mol]:	112.21
CAS:	39782-43-9

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	38.10	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	712.50		NIST Webbook
rinpol	709.50		NIST Webbook
rinpol	706.20		NIST Webbook
rinpol	712.50		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	716.80		NIST Webbook
tb	377.30 ± 0.50	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.23577e+01
Coeff. B	-2.53285e+03
Coeff. C	-6.60830e+01
Temperature range (K), min.	275.93
Temperature range (K), max.	425.55

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

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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