

trans-4,4-Dimethyl-2-hexene

Other names:	(2E)-4,4-Dimethyl-2-hexene (E)-2-Hexene, 4,4-dimethyl (E)-4,4-Dimethylhex-2-ene 2-Hexene, 4,4-dimethyl, trans 4,4-Dimethyl-trans-2-hexene
Inchi:	InChI=1S/C8H16/c1-5-7-8(3,4)6-2/h5,7H,6H2,1-4H3/b7-5+
InchiKey:	OQEVAISXHCRRGF-FNORWQNLSA-N
Formula:	C8H16
SMILES:	CC=CC(C)(C)CC
Mol. weight [g/mol]:	112.21
CAS:	19550-83-5

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	724.90		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	748.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	735.00		NIST Webbook
tb	383.37	K	Joback Method
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/molxK	383.37	Joback Method
cpg	233.64	J/molxK	413.94	Joback Method
cpg	247.38	J/molxK	444.50	Joback Method
cpg	260.39	J/molxK	475.07	Joback Method
cpg	272.68	J/molxK	505.64	Joback Method
cpg	284.31	J/molxK	536.21	Joback Method
cpg	295.30	J/molxK	566.77	Joback Method
dvisc	0.0110015	Paxs	177.26	Joback Method
dvisc	0.0034054	Paxs	211.61	Joback Method
dvisc	0.0014626	Paxs	245.96	Joback Method
dvisc	0.0007728	Paxs	280.31	Joback Method
dvisc	0.0004693	Paxs	314.67	Joback Method
dvisc	0.0003144	Paxs	349.02	Joback Method
dvisc	0.0002263	Paxs	383.37	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.25062e+01
Coeff. B	-2.58614e+03
Coeff. C	-6.54900e+01
Temperature range (K), min.	277.15
Temperature range (K), max.	424.94

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550835&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

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

Latest version available from:

<https://www.cheméo.com/cid/65-125-1/trans-4-4-Dimethyl-2-hexene.pdf>

Generated by Cheméo on 2024-04-23 11:02:21.408587106 +0000 UTC m=+16159390.329164442.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.