5-Methyl-3-heptene

Other names: 5-Methyl-trans-3-heptene
Inchi: InChI=1S/C8H16/c1-4-6-7-8(3)5-2/h6-8H,4-5H2,1-3H3
InchiKey: YMNTZRCUPAYGLG-UHFFFAOYSA-N
Formula: C8H16
SMILES: CCC=CC(C)CC
Mol. weight [g/mol]: 112.21
CAS: 53510-18-2

Physical Properties

Property code	Value	Unit	Source
gf	94.26	kJ/mol	Joback Method
hf	-96.51	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	38.90	kJ/mol	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.999		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	386.16	K	Joback Method
tc	562.05	K	Joback Method
tf	159.84	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.94	J/mol×K	386.16	Joback Method
cpg	231.23	J/mol×K	415.47	Joback Method
cpg	243.94	J/mol×K	444.79	Joback Method
cpg	256.10	J/mol×K	474.10	Joback Method
cpg	267.72	J/mol×K	503.42	Joback Method
cpg	278.83	J/mol×K	532.73	Joback Method
cpg	289.43	J/mol×K	562.05	Joback Method
dvisc	0.0101457	Pa×s	159.84	Joback Method

dvisc	0.0028001	Pa×s	197.56	Joback Method
dvisc	0.0011677	Pa×s	235.28	Joback Method
dvisc	0.0006201	Pa×s	273.00	Joback Method
dvisc	0.0003840	Pa×s	310.72	Joback Method
dvisc	0.0002638	Pa×s	348.44	Joback Method
dvisc	0.0001950	Pa×s	386.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41614e+01
Coeff. B	-3.29361e+03
Coeff. C	-4.82220e+01
Temperature range (K), min.	285.62
Temperature range (K), max.	420.39

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53510182&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/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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume