3-Heptene, 4-methyl-

Other names:	4-Methyl-3-heptene
Inchi:	InChI=1S/C8H16/c1-4-6-8(3)7-5-2/h6H,4-5,7H2,1-3H3
InchiKey:	KKVVJQGDNYIIMN-UHFFFAOYSA-N
Formula:	C8H16
SMILES:	CCC=C(C)CCC
Mol. weight [g/mol]:	112.21
CAS:	4485-16-9

Physical Properties

Property code	Value	Unit	Source
gf	88.15	kJ/mol	Joback Method
hf	-101.02	kJ/mol	Joback Method
hfus	15.37	kJ/mol	Joback Method
hvap	33.44	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.143		Crippen Method
mcvol	119.280	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
tb	386.48	K	Joback Method
tc	561.75	K	Joback Method
tf	160.88	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.03	J/mol×K	386.48	Joback Method
cpg	231.15	J/mol×K	415.69	Joback Method
cpg	243.70	J/mol×K	444.90	Joback Method
cpg	255.70	J/mol×K	474.11	Joback Method
cpg	267.18	J/mol×K	503.32	Joback Method
cpg	278.15	J/mol×K	532.54	Joback Method
cpg	288.64	J/mol×K	561.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50472e+01
Coeff. B	-3.57324e+03
Coeff. C	-5.07240e+01
Temperature range (K), min.	292.82
Temperature range (K), max.	417.75

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4485169&Units=SI

Legend

cpg:	Ideal gas heat capacity
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

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